Construction of Optimal Parameters for the Test Particle Monte Carlo Method

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The test particle Monte Carlo method for solving the linearized Boltzmann equation is considered. The main idea of this work is the construction of the relations between the sample size and the number of grid nodes which guarantee the attainment of the given error level on the base of the theory of discrete-stochastic numerical methods. Two approaches to construction of the upper error bound of the method are suggested. The optimal (in the sense of the obtained upper error bounds) relations between the sample size and the number of grid nodes are constructed.

Keywords: test particle Monte Carlo method, optimization, error bond, discrete-stochastic methods.
PACS: 02.70.Uu, 02.60.-x, 02.70.-c

Introduction.

Since 60-th the Monte Carlo method has being actively used to solve the Boltzmann equation [1,2]. A whole series of approaches for solving the Boltzmann equation taking into account specific characters of concrete problems have been developed. Frequently under simulation the flow of gases mixture with a small concentration of one of the components it is possible to neglect collisions of test particles with each other and their influence on the background gas. For solving such problems, the so-called test particle Monte Carlo method [2,3] is used. The test particle Monte Carlo method consists in simulation of test particle trajectories in a background gas. All necessary macroparameters of test particle flow (functionals of the distribution function) are computed during the trajectory simulation. In practice as a rule one is interested in spatial distribution of flow macroparameters. Usually some grid is constructed in the interesting domain, then flow macroparameters are estimated in the grid nodes and some interpolation procedure is applied. Thus one needs to choice the number of grid nodes and the sample size to construct approximation of macroparameters on the domain in whole with some given error level. As a rule control of statistical and deterministic errors is realized independently of one another. In recent time the theory of discrete-stochastic numerical methods has been developed for different problems [4 - 11]. This theory allows doing the choice of the number of grid nodes and the sample size by an optimal way.

The aim of the presented article is application of the discrete-stochastic approaches to solving the linearized Boltzmann equation by the test particle Monte Carlo method.

In the presented work we consider two types of stochastic estimators for this method. They are the intersection estimator and the time estimator. When using the intersection estimator, the summation of data required for the calculation of gas macroparameters in a point $\mathbf{x}$ occurs during the motion of the particles, and the necessary values are determined at a preset plane with coordinate $\mathbf{x}$. As soon as a particle crosses such a plane, the summation of the information with a weight $\mathbf{1/v_x}$ happens (here $\mathbf{v_x}$ is the particle velocity in the direction perpendicular to the plane) [3]. For the time estimator the information is summed to cells that a particle passed through, and the contribution of a particle is proportional to the time that the particle stays in the cell. Note that the time estimator is analogue of the path estimator, which is actively used for solving of problems in the transport theory [4,10].

1. Discrete-Stochastic Numerical Methods

Since recently, approaches have been developed for construction and optimization of the Monte Carlo algorithms for an approximation on domain in whole a solution of some equation [4-11]. These approaches are connected with preliminary discretization of the problem (introduction of a grid), estimation of a solution at the grid nodes by the Monte Carlo method, and subsequent interpolation of the solution from the so-obtained approximate values at the nodes.

A peculiarity of numerical methods under study is the presence of deterministic and stochastic components of the error, which leads to some difficulties in convergence studying and optimization of these procedures. The main difficulty resides in construction of the upper bounds for the stochastic error component. Here important moments are the properties of the corresponding interpolation as well as the peculiarities of the stochastic estimators for the values of a solution at nodes, namely, dependent, independent, or weakly dependent estimators. Another important problem is to choose optimal values of the parameters of discrete-stochastic numerical methods, namely, the number of grid nodes and the sample size. Here we use the optimization approach of works [4,6]. We suppose that the upper error bound reproduces the dependence of the error on parameters quite precisely and we equate this bound to a prescribed error level. Under this condition, we minimize the cost function whose arguments are the sought parameters.

Thus let **u** denotes one of the flow macroparameters which is to be approximated as a function on some bounded domain **D.** Then the discrete-stochastic numerical method looks as follows.

1. Construct a grid $\{r^{(i)}\}_{i=1}^{M}$ in the domain **D**.

2. Use the Monte Carlo algorithm to evaluate the values of the solution at the grid nodes:

$$u(r^{(i)}) \approx \widetilde{u}(r^{(i)}) = 1/N \sum_{n=1}^{N} \xi_n^{(i)},$$

where $\xi_n^{(i)}$ are independent samples of $\xi^{(i)}$ (n=1,…,N), and $\xi^{(i)}$ is a random estimator of $u(r^{(i)})$, i.e. $E\xi^{(i)} = u(r^{(i)})$ (or $E\xi^{(i)} \approx u(r^{(i)})$ for biased estimator).

3. Apply an interpolation procedure, which uses the values obtained at the grid nodes $\widetilde{u}(r^{(i)})$ to evaluate u as a function on **D**:

$$u(r) \approx L_{(M)}\widetilde{u}(r) = \sum_{i=1}^{M} \widetilde{u}(i)\chi_i(r), \qquad (1.1)$$

where $\chi_i(r)$ are basis functions of interpolation. In what follows we consider only linear interpolation.

We need to construct the optimal relation between the sample size N and the number of grid nodes M. For this purpose we have to carry out two steps as in works [6,8-11]:

1. To construct the upper error bound in the metric of continuous function space **C** with convergence in probability, i.e., the relation of the following type

$$P\left\{\delta = \sup_{x\in D}\left|u(r) - L_M\widetilde{u}(r)\right| \le T(M,N)\right\} > 1-\theta,$$

where $T(M,N)\to 0$ as $M,N\to\infty$ and $\theta>0$ is a small value.

2. To solve the optimization problem of the following type:

$$\min_{M,N} S(M,N) \quad \text{provided that} \quad T(M,N) = \alpha \qquad (1.2)$$

where $S(M,N)$ is a cost function, $T(M,N)$ is the upper bound of the error and $\alpha>0$ is some fixed error level.

2. Upper Error Bound

Let us consider the error of approximation (1.1) in the metric of continuous function space **C**, i.e., the quantity

$$\delta = \sup_{r\in D}\left|u(r) - L_{(M)}\widetilde{u}(r)\right|. \qquad (2.1)$$

According to the triangle inequality the error (2.1) is expanded into three components. They are: the interpolation component, the bias, and the stochastic component:

$$\delta \le \sup_{r\in D}\left|u(r)-L_{(M)}u(r)\right| + \sup_{r\in D}\left|L_{(M)}u(r)-L_{(M)}\mathbb{E}\tilde{u}(r)\right| + \sup_{r\in D}\left|L_{(M)}\mathbb{E}\tilde{u}(r)-L_{(M)}\tilde{u}(r)\right| = \delta_1+\delta_2+\delta_3 \quad (2.2)$$

Here the following notations are used $L_{(M)}u(r)=\sum_{i=1}^{M}u(r^{(i)})\chi_i(r)$, $L_{(M)}\mathbb{E}\tilde{u}(r)=\sum_{i=1}^{M}E\xi^{(i)}\chi_i(r)$.

The first two error components in (2.2) are deterministic while the third one is random.

The first summand δ_1 is the error of the linear interpolation. Provided that corresponding conditions are satisfied, the error of the linear interpolation has the second order on the grid step. For instance if u ∈ $\mathbf{C}^{(2)}$(D), then there exists a positive constant H_I such that the following inequality holds [12] $\delta_1 \le H_I M^{-2}$ (2.3)

The second term in (2.2) corresponds to the bias. For linear interpolation the error concentrates at the grid nodes, i.e. the following equality holds [5,6] $\delta_2 \le \max_{i=1,\dots,M}\left|u(r^{(i)})-E\xi^{(i)}\right|$. Here $\left|u(r^{(i)})-E\xi^{(i)}\right|$ is the value of the bias at the *i*-th node.

The bias at the node for algorithm with the time estimators has the second order on the grid step as for the algorithm with the path estimators [10]. So if $u \in \boldsymbol{C}^{(2)}(D)$, then there exists a positive constant H_B such that the following inequality holds $\delta_2 \le H_B M^{-2}$ (2.4)

The bias at the node for algorithm with the intersection estimators has another character. The point is that the intersection estimator has the infinite variance and usually the modified intersection estimator with finite variance is used. For such estimator the summation of the information with a weight $1/v_x$ happens only if $|v_x| > \varepsilon$ (here v_x is the velocity of the particle in the direction perpendicular to the plane, ε is some given small value). In this case we have the ε-biased estimator at the node and the value of its bias has the first order on ε [4]. So we obtain the following upper bound for the bias component $\delta_2 \le \widetilde{H}_B\varepsilon$ (2.5)

The third summand in (2.2) is the stochastic component of the error. The following inequality takes place $P\{\ \delta_3 \le \sqrt{\frac{H_V}{N}}\max_{i=1,\dots,M}\left|\gamma^{(i)}\right|\ \} > 1-\theta,$ where $\gamma^{(i)}$ are the jointly normal standard random variables [6-11]. The main difficulty consists in estimating of the maximum $\max_{i=1,\dots,M}\left|\gamma^{(i)}\right|$. By taking into account the properties of the used estimators at the grid nodes (namely, independent, weakly dependent, or dependent-trials estimators), sufficiently accurate upper bounds for such maximums were constructed in [5,6,8,11,13]. For both considered algorithms estimators at the grid nodes are strongly dependent and so to construct the upper bounds for the stochastic error components we suggest two approaches:

1) The first universal approach is suitable under any dependencies between estimators at the grid nodes. It was proposed in work [13]. Note that the more information about correlations between estimators we have, the more exact upper bound for the stochastic error component we can construct. In this respect the first approach does not require any information about correlations, but the so constructed upper bound turns out somewhat overestimated. In this approach upper bound τ_M of maximum of *M* normal standard random variables is constructed in the form

$$\tau_M = \Phi_{0,1}^{-1}(1-\theta/(4M)),$$

where $\Phi_{0,1}$ is the standard normal distribution function. For simplicity τ_M is approximated by power function μM^{ν}, where *ν* is a small value.

2) The second approach is based on the selection of some stationary Gaussian zero mean and unit variance process with correlation function which approximates the correlation matrix of jointly normal standard random variables $\{\gamma^{(i)}\}_{i=1}^{M}$ [11]. We suggest to use stationary Gaussian zero mean and unit variance processes with analytically known distribution of $sup_{r\in D}|\gamma(r)|$ for this purpose. In particular, the examples of such processes are presented in works [14,15]. It is known that the stationary Gaussian zero mean and unit variance process is uniquely determined by its correlation function. We build correlation matrix of the jointly normal standard random variables $\{\gamma^{(i)}\}_{i=1}^{M}$ on the base of preliminary computations [11] and then select a stationary Gaussian zero mean and unit variance process whose correlation function approximates this correlation matrix with some accuracy.

Upper error bound for algorithm with the time estimators.

By summing above reasoning we represent the upper error bounds for algorithm with the time estimators at first. Later *mes* ***D*** denotes Lebesgue measure of the domain **D**.

First approach $$P\{\delta \le \frac{H_1}{M^2} + \frac{H_2}{\sqrt{N}}\mu M^{\nu}\} > 1-\theta \quad (2.6)$$

Second approach $$P\{\delta \le \frac{H_1}{M^2} + \frac{H_2(\theta)}{\sqrt{N}}\} > 1-\theta \quad (2.7)$$

Upper error bound for algorithm with the intersection estimators.

In this subsection we represent the corresponding upper error bounds for algorithm with the intersection estimators.

First approach $$P\{\delta \le \frac{\widetilde{H}_1}{M^2} + \widetilde{H}_0\varepsilon + \frac{\widetilde{H}_2(\varepsilon)}{\sqrt{N}}\mu M^{\nu}\} > 1-\theta \quad (2.8)$$

Second approach $$P\{\delta \le \frac{\widetilde{H}_1}{M^2} + \widetilde{H}_0\varepsilon + \frac{\widetilde{H}_2(\varepsilon,\theta)}{\sqrt{N}}\} > 1-\theta \quad (2.9)$$

Here

$H_1 = mes^2 D\|u''\|_\infty/6,\ \widetilde{H}_1 = mes^2 D\|u''\|_\infty/8,\ H_2 = \sqrt{\max_i V\xi^{(i)}},\ H_2(\theta) = G(\theta)\sqrt{\max_i V\xi^{(i)}},$

$\widetilde{H}_2(\varepsilon) = \sqrt{\max_i V\xi^{(i)}(\varepsilon)}$, $\widetilde{H}_2(\varepsilon,\theta) = G(\theta)\sqrt{\max_i V\xi^{(i)}(\varepsilon)},$ $G(\theta)$ is the estimate of the selected Gaussian process maximum.

3. The Optimization Problem

The upper error bounds (2.6) - (2.9) can be used to set the series of optimization problems: find the values M_{opt}, N_{opt} (and ε_{opt} for algorithm with the intersection estimators only) that minimize the algorithm computational cost under a given error level α, i.e. problem (1.2), where T(M,N) is the upper error bound from (2.6) - (2.9). Here the computational cost is proportional to the number of trajectories and the number of grid nodes: $S(M,N) = t_0 NM$.

This series of optimization problems is solved similarly with one from work [10]. Later we present the optimal (with regard to the upper error bound) values of parameters and corresponding to them computational cost.

Algorithm with the time estimators. First approach.

$$M_{opt} = (\frac{5+2\nu}{1+2\nu}H_1)^{1/2}\alpha^{-1/2},\ N_{opt} = (\frac{5+2\nu}{4}H_2\mu M_{opt}^{\nu})^2\alpha^{-2},\ S_{opt} \sim \alpha^{-5/2}(-\ln\alpha). \quad (3.1)$$

Algorithm with the time estimators. Second approach.

$$M_{opt} = (5H_1)^{1/2}\alpha^{-1/2},\ N_{opt} = (5H_2/4)^2\alpha^{-2},\ S_{opt} \sim \alpha^{-5/2} \quad (3.2)$$

Algorithm with the intersection estimators. First approach.

$$\varepsilon_{opt} = \frac{2\alpha}{(5+2\nu)H_0|\ln\alpha|},\ M_{opt} = (\frac{(5+2\nu)H_1}{(1+2\nu)(1-2((5+2\nu)|\ln\alpha|)^{-1})})^{1/2}\alpha^{-1/2},$$

$$N_{opt} = (\frac{5+2\nu}{4(1-2((5+2\nu)|\ln\alpha|)^{-1})}H_2\mu M_{opt}^{\nu})^2\alpha^{-2},\ \ S_{opt} \sim \alpha^{-5/2}(-\ln\alpha). \quad (3.3)$$

Algorithm with the intersection estimators. Second approach.

$$\varepsilon_{opt} = \frac{\alpha}{2H_0|\ln\alpha|}, M_{opt} = (\frac{5H_1}{1-(2|\ln\alpha|)^{-1}})^{1/2}\alpha^{-1/2}, N_{opt} = (\frac{5H_2}{4(1-(2|\ln\alpha|)^{-1}})^2\alpha^{-2}\ S_{opt} \sim \alpha^{-5/2} \quad (3.4)$$

Note those values μ and ν are needed to calculate the optimal values of parameters for the first approach. The following algorithm is used to estimate them [13]:

1) Value $M_{opt}^{(0)}$ is calculated under $\nu = 0$. 2) Approximation of τ_M by power function is constructed in some neighborhood of point $M_{opt}^{(0)}$ and the corresponding values μ_1 and ν_1 are calculated. 3) Value $M_{opt}^{(1)}$ is calculated

under $\nu = \nu_1$. 4) If $M_{opt}^{(1)}$ differ from $M_{opt}^{(0)}$ greatly then approximation of τ_M by power function is constructed again for new point $M_{opt}^{(1)}$, new values μ_2 and ν_2 are calculated and so on. Otherwise obtained values μ_i and ν_i are used to calculate the optimal values of parameters.

4. Numerical Experiments

We study the availability of the obtained optimal values of parameters on the example of the classical problem of heat transfer between two parallel plates. The physical formulation of the problem is as follows. The background gas with an average density n_0 is confined between two rigid infinite plates positioned at the planes $z=0$ and $z=D$. The temperatures of the lower and upper plates (T_0 and T_D respectively) are constant. The reflection from the plates is taken diffuse with a complete accommodation of momentum and energy. The hard sphere model [1] is employed for the description of intermolecular collisions. One has to determine the gas macroparameters between the plates under given temperatures T_0, T_D and the degree of gas rarefaction [1]. For characterization of gas rarefaction, we use the Knudsen number $Kn=L/D$. Here L is the mean free path of test particles in the background gas.

The calculations are carried out under the following problem parameters: $T_0/T_D = 0.25$, $Kn = 1$. Density and temperature of the background gas are constant (n_0 and T_0 correspondingly) over the whole domain. The density of the test particles on the whole domain is calculated. A test solution computed with a high accuracy is used for evaluating the obtained errors instead of the unknown exact solution. The optimal values of the parameters are determined by the formulas (3.1) - (3.4). At that all necessary constants are estimated on the base of preliminary computations. In second approach we used the stationary Gaussian process from work [11].

The calculation results for different error levels α with using of the optimal values of the parameters corresponding to two suggested approaches are given in tables 1,2 (for algorithm with the time estimators) and in tables 3,4 (for algorithm with the intersection estimators).

The following notations are used in the tables. Through $\delta_i, \delta_s, \delta$ we denote the interpolation, stochastic, and total errors, respectively. The stochastic error δ_s is evaluated as the maximum of the absolute value of the difference between the «exact» and approximate solutions at the nodes and so it includes the bias too. The error of interpolation δ_i is evaluated by using the difference between the «exact» solution and the solution interpolated over the «exact» values in the grid nodes at 10^6 random points from D. The total error δ is the sum of the interpolation error δ_i and the stochastic error δ_s. The value σ serves for control of the stochastic error. It is evaluated as $\max_{i=1,\dots,M} \sqrt{V\xi^{(i)}/N}$, where $V\xi^{(i)}$ is the sample variance. t is the computer time in seconds used to calculate the approximate solution in the grid nodes.

TABLE 1. Algorithm with the time estimators. First approach

$\alpha\times10^2$	N_{opt}	M_{opt}	$\sigma\times10^2$	$\delta_i\times10^2$	$\delta_s\times10^2$	$\delta\times10^2$	t
5	28350	44	3.237	1.265	2.050	3.315	1.3
2.5	119752	62	1.633	0.855	1.156	2.011	6.94
1	801871	98	0.644	0.474	0.445	0.919	66.38
0.5	3369919	139	0.322	0.238	0.186	0.424	375.19
0.25	14139602	197	0.161	0.092	0.072	0.164	2148.64

TABLE 2. Algorithm with the time estimators. Second approach

$\alpha\times10^2$	N_{opt}	M_{opt}	$\sigma\times10^2$	$\delta_i\times10^2$	$\delta_s\times10^2$	$\delta\times10^2$	t
5	32257	47	3.050	1.187	2.092	3.279	1.53
2.5	129028	66	1.583	0.795	1.244	2.039	7.81
1	806422	104	0.644	0.441	0.500	0.941	70.69
0.5	3225685	146	0.330	0.213	0.212	0.425	375.81
0.25	12902737	207	0.169	0.081	0.078	0.159	2051.34

TABLE 3. Algorithm with the intersection estimators. First approach.

$\alpha\times10^2$	$\varepsilon_{opt}\times10^3$	N_{opt}	M_{opt}	$\sigma\times10^2$	$\delta_i\times10^2$	$\delta_s\times10^2$	$\delta\times10^2$	t
5	3.58	29677	41	3.244	1.359	1.519	2.878	1.81
2.5	1.46	137447	57	1.570	0.942	1.136	2.078	10.81
1	0.468	1030677	89	0.602	0.531	0.438	0.969	117.8
0.5	0.204	4685303	125	0.300	0.311	0.136	0.447	724.8
0.25	0.090	21171514	176	0.146	0.133	0.092	0.225	4488

TABLE 4. Algorithm with the intersection estimators. Second approach.

$\alpha\times10^2$	$\varepsilon_{opt}\times10^3$	N_{opt}	M_{opt}	$\sigma\times10^2$	$\delta_i\times10^2$	$\delta_s\times10^2$	$\delta\times10^2$	t
5	4.636	35591	44	2.974	1.266	1.643	2.909	2.30
2.5	1.883	154395	61	1.490	0.872	0.839	1.711	12.82
1	0.603	1072054	95	0.591	0.491	0.370	0.861	130.3
0.5	0.262	4621807	133	0.297	0.267	0.147	0.414	755.0
0.25	0.116	19835610	187	0.150	0.110	0.115	0.225	4440

Conclusion

1) The test particle Monte Carlo method (with the time and intersection estimators) for solving the linearized Boltzmann equation is considered. The main idea of this work is the construction of the relations between the sample size and the number of grid nodes which guarantee the attainment of the given error level on the base of the theory of discrete-stochastic numerical methods.

2) For this purpose we suggest two approaches to construction of the upper error bounds which take into account information about dependencies between estimators at the grid nodes.

3) The optimal (in the sense of obtained upper error bounds) relations between the sample size and the number of grid nodes are constructed.

4) The numerical results presented in the tables show that for every approach and for both algorithms, the total error δ does not exceed the permissible error level α if we use optimal values of the parameters.

5) At that the calculating time for the algorithm with time estimators is somewhat less then one for the algorithm with intersection estimators.

6) The comparison of the formulas (3.1) - (3.4) shows that the second approach has the least computational cost asymptotically as $\alpha\to0$. The numerical experiments confirm this theoretical result.

7) Note that the first approach does not need any information about dependencies between estimators.

ACKNOWLEDGMENTS

The work was partially supported by RFBR (grant N 06-01-00046) and by grant of President of the Russian Federation for support of the Leading Scientific Schools (N 4774.2006.1).

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