A New Class of Grid-Free Monte Carlo Algorithms for Elliptic Boundary Value Problems*

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Abstract. In this paper we consider the following mathematical model: an elliptic boundary value problem, where the partial differential equation contains advection, diffusion, and deposition parts. A Monte Carlo (MC) method to solve this equation uses a local integral representation by the Green's function and a random process called "Walks on Balls"(WOB). A new class of grid free MC algorithms for solving the above elliptic boundary value problem is suggested and studied. We prove that the integral transformation kernel can be taken as a transition density function in the Markov chain in the case when the deposition part is equal to zero. An acceptance-rejection (AR) and an inverse-transformation methods are used to sample the next point in the Markov chain. An estimate for the efficiency of the AR method is obtained.

1 Formulation of the Problem

Consider the functional

$$J(u) \equiv (g,u) = \int_{\Omega} g(x)u(x)dx, \tag{1}$$

where $\Omega \subset R^3$ and $x = (x_1, x_2, x_3) \in \Omega$ is a point in the Euclidean space R^3. The functions $u(x)$ and $g(x)$ belong to the Banach space X and to the adjoint space X^*, respectively, and $u(x)$ is a unique solution of the following Fredholm integral equation:

$$u(x) = \int_{\Omega} k(x,y)u(y)dy + f(x). \tag{2}$$

The main task is to calculate the functional (1), where $u(x)$ is the solution of the following boundary value problem:

$$Mu = -\Phi(x), \qquad x \in \Omega, \quad \Omega \subset R^3, \tag{3}$$

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$$u = \psi(x), \qquad x \in \partial\Omega, \tag{4}$$

where the operator M is defined by: $M = \sum_{i=1}^{3} \left(\frac{\partial^2}{\partial x_i^2} + b_i(x) \frac{\partial}{\partial x_i} \right) + c(x)$.

As shown in [1,7], if the coefficients of the operator M satisfy the conditions: $b_i(x)$, $c(x) \in C^{(0,\lambda)}(\overline{\Omega})$, $c(x) \leq 0$, $\Phi \in C^{(0,\lambda)}(\Omega) \bigcap C(\overline{\Omega})$ and $\psi \in C(\partial\Omega)$ in the closed domain $\overline{\Omega} \in A^{(1,\lambda)}$, then the problem (3) - (4) has an unique solution $u(x) \in C^2(\Omega) \bigcap C\left(\overline{\Omega}\right)$. A definition for the class $A^{(k,\lambda)}$ can be found in [6].

We denote by $B(x)$ the maximal ball inside the domain Ω with radius $R(x)$ and center in the point x, i.e.:

$$B(x) = B_{R(x)} = \{ y : r = |y - x| \leq R(x) \}. \tag{5}$$

Levy's function for the problem (3)-(4) [8] is:

$$L_p(y, x) = \mu_p(R) \int_r^R \left(\frac{1}{r} - \frac{1}{\rho} \right) p(\rho) d\rho, \quad r \leq R, \tag{6}$$

where $p(r)$ is a density function and the following notation is used:

$$r = |x - y| = \left(\sum_{i=1}^{3} (x_i - y_i)^2 \right)^{1/2}, \quad \mu_p(R) = (4\pi q_p(R))^{-1}, \quad q_p(R) = \int_0^R p(\rho) d\rho.$$

The components of the vector-function $\mathbf{b}(x)$ are assumed to satisfy the conditions: $b_i(x) \in C^{(1)}(\Omega), i = 1, 2, 3$ and $div\mathbf{b}(x) = 0$. Then a local integral representation of the solution by the use of the Green's function approach exists for standard domains, lying inside Ω. In addition, taking in account that $\frac{\partial L_p(y,x)}{\partial y_i} = \mu_p(R) \frac{x_i - y_i}{r^3} \int_r^R p(\rho) d\rho$, one can see that the Levy's function satisfies the conditions:

$$\frac{\partial L_p(y, x)}{\partial y_i} = L_p(y, x) = 0 \quad \text{for any} \quad y \in \partial\Omega. \tag{7}$$

Finally, the solution of the problem (3)-(4) can be written in the following integral form [4,8]:

$$u(x) = \int_{B(x)} M_y^* L_p(y, x) u(y) dy + \int_{B(x)} L_p(y, x) \Phi(y) dy, \tag{8}$$

where $M^* = \sum_{i=1}^{3} \left(\frac{\partial^2}{\partial x_i^2} - b_i(x) \frac{\partial}{\partial x_i} \right) + c(x)$ is the adjoint operator to M and

$$M_y^* L_p(y, x) = \mu_p(R) \frac{p(r)}{r^2} - \mu_p(R) c(y) \int_r^R \frac{p(\rho)}{\rho} d\rho$$

$$+ \frac{\mu_p(R)}{r^2} \left[c(y) r + \sum_{i=1}^{3} b_i(y) \frac{y_i - x_i}{r} \right] \int_r^R p(\rho) d\rho. \tag{9}$$

The MC method, that solves our problem uses the local integral representation (8) and a WOB random process.

2 Monte Carlo Algorithms

The Monte Carlo estimator with mathematical expectation equal to $J(u)$ is

$$\Theta[g] = \frac{g(\xi_0)}{\pi(\xi_0)} \sum_{j=0}^{\infty} Q_j f(\xi_i), \tag{10}$$

where $Q_0 = 1, Q_j = Q_{j-1} \frac{k(\xi_{j-1},\xi_j)}{p(\xi_{j-1},\xi_j)}, j = 1, 2, 3, ...$, and $\xi_0, \xi_1, ...$ is a Markov chain in Ω with initial density function $\pi(x)$ and transition densities $p(x, y)$, which are tolerant to $g(x)$ and $k(x, y)$, respectively (see [2,5,9]).

To ensure the convergence of the process, we introduce an ε - strip of the boundary. The process starts at point $\xi_0 = x \in \Omega$, which is chosen correspondingly with the initial density function $\pi(x)$. The next random point is determined by a transition density function $p(x, y)$. This process terminates when the point falls into the ε - strip of the boundary.

The kernel, $k(x, y) = M_y^* L_p(y, x)$, of the integral equation (8) can be used as a transition density in the Markov chain when it is non-negative. This condition is satisfied in the case when the density function $p(r) = e^{-kr}$ and $k = b^* + \overline{R}c^*$, where $b^* = \max_{x\in\Omega} \mid \mathbf{b}(x) \mid$, $c^* = \max_{x\in\Omega} \mid c(x) \mid$, and $\overline{R}$ is the radius of the maximal ball lying inside Ω [3,4].

Here we propose and study new MC algorithms, where the density function $p(r)$ depends only on the advection part $\mathbf{b}(x)$ of the elliptic equation.

The following assertion holds:

Theorem 1. *If for the function $p(r) \geq 0$ the inequality*

$$p(r) \geq b^* \int_r^R p(\rho) d\rho \tag{11}$$

is true, then the function

$$p(x, y) = \frac{\mu_p(R)}{r^2} \left[p(r) + \sum_{i=1}^{3} b_i(y) \frac{y_i - x_i}{r} \int_r^R p(\rho) d\rho \right] \tag{12}$$

can be used as a transition density for Markov process.

Proof. The function (12) is obtained from the kernel $k(x, y)$ when $c(y) \equiv 0$. It is already proved in [4] that $\int_{B(x)} p(x, y) dy = 1$. The remaining task is to find out when $p(x, y) \geq 0$.

By using spherical coordinates:

$$y_1 - x_1 = r\sin\theta\sin\varphi, \quad y_2 - x_2 = r\sin\theta\cos\varphi, \quad y_3 - x_3 = r\cos\theta,$$

and replacing $\omega_i = (y_i - x_i)/r$, the following equations hold:

$$\sum_{i=1}^{3} b_i(y)\frac{y_i - x_i}{r} = \sum_{i=1}^{3} b_i(x + r\mathbf{w})\omega_i = (\mathbf{b}, \mathbf{w}). \tag{13}$$

From the inequalities $|(\mathbf{b}, \mathbf{w})| \leq |\mathbf{b}||\mathbf{w}| = |\mathbf{b}| \leq b^*$ we obtain the estimate $\sum_{i=1}^{3} b_i(y)(y_i - x_i)/r \geq -b^*$, and finally:

$$p(x, y) \geq \frac{\mu_p(R)}{r^2}\left[p(r) - b^* \int_r^R p(\rho)d\rho\right]. \tag{14}$$

The proof is completed as (14) leads to (11). $\diamond$

This theorem gives us the base for new class MC algorithms, where the choice of $p(r)$ depends only on b^* and does not depend on c^* and $\overline{R}$.

The function $p(x, y)$ can be written in spherical coordinates as:

$$p(r, \mathbf{w}) = \frac{\sin\theta}{4\pi}\frac{p(r)}{q_p(R)}\widetilde{p}(\mathbf{w}|r), \quad \widetilde{p}(\mathbf{w}|r) = 1 + \frac{|\mathbf{b}(x + r\mathbf{w})|\cos(\mathbf{b}, \mathbf{w})}{p(r)}\int_r^R p(\rho)d\rho.$$

Now, the next random point y in the Markov chain depends on the direction $\mathbf{w}$ and on the jump r that is made to an internal point into the maximal ball. First we sample the random jump r with density function $p(r)/q_p(r)$ using an inverse-transformation method. To obtain the random direction $\mathbf{w}$ with density function $p(\mathbf{w}|r) = \frac{\sin\theta}{4\pi}\widetilde{p}(\mathbf{w}|r)$ an acceptance-rejection (AR) method is used.

Since $\widetilde{p}(\mathbf{w}|r) \leq \left[1 + \frac{b^*}{p(r)}\int_r^R p(\rho)d\rho\right] = h(r)$, the function $h(r)$ can be accepted as a majorant for the AR method.

Here, the algorithm for one random walk is described:

1. **Calculate** the radius $R(x)$.
2. **Sample** the jump r with density $\frac{p(r)}{q_p(R)}$.
3. **Calculate** the function $h(r)$.
4. **Compute** the independent realizations $\mathbf{w_j}$ of a unit isotropic vector in $\mathbf{R}^3$.
5. **Compute** the independent realizations γ_j of a uniformly distributed random variable in the interval $[0, 1]$.
6. **Repeat** the steps 4 and 5 until define the parameter j_0 from the condition: $j_0 = \min\{j : h(r)\gamma_j \leq \widetilde{p}(\mathbf{w_j}|r)\}$. The random vector $\mathbf{w_{j_0}}$ has the density $p(\mathbf{w}|r)$.
7. **Calculate** the next random point y by formula $y = x + r\mathbf{w_{j_0}}$.
8. **Stop** the algorithm when the random process reaches the ε -strip of the boundary. If $y \notin \partial\Omega_\varepsilon$ then the algorithm has to be repeated for $x = y$.

We consider and analyze three possible alternatives for the density function $p(r)$:

$\bullet p(r) = e^{-b^* r}$ $\bullet p(r) = const.$ $\bullet p(r) = e^{b^* r}$

In the first case, when $p(r) = e^{-b^* r}$ we have:

$$b^* \int_r^R p(\rho) d\rho = e^{-b^* r} - e^{-b^* R} \leq e^{-b^* r}.$$

Therefore the inequality (11) is always true. The following assertion holds:

Lemma 1. *If $p(r) = e^{-b^* r}$ then the function $p(x, y)$ can be used as a transition density.*

The advantage of such kind of choice is that it does not depend on any additional requirements to the parameters of the problem.

In the second case, when $p(r) = const.$, the inequality (11) is equivalent to: $b^*(R - r) \leq 1$. From $0 \leq r \leq R$ follows: $b^*(R - r) \leq b^* R \leq b^* \overline{R}$. Thus we can formulate the conclusion:

Lemma 2. *If the parameters of the problem satisfy the inequality*

$$b^* \overline{R} \leq 1 \tag{15}$$

and the density function $p(r)$ is chosen to be $p(r) = const.$, then the function $p(x, y)$ can be used as a transition density.

Because of the computational simplicity, one can expect that the use of a constant density leads to decreasing of the computational cost of the algorithm in comparison with the algorithms, using exponential densities.

In the third case, when $p(r) = e^{b^* r}$, the inequality (11) is true when: $b^*(R - r) \leq \ln 2$. Finally, we reached to the assertion:

Lemma 3. *If the parameters of the problem satisfy the inequality*

$$b^* \overline{R} \leq \ln 2 \tag{16}$$

and the density function $p(r)$ is chosen to be $p(r) = e^{b^* r}$, then the function $p(x, y)$ can be used as a transition density function in Markov process.

Since the function $e^{b^* r}$ is strictly increasing, the choice of a bigger jump r in the ball in the Markov chain is more probable. One can expect that the average moves (El_ε) in the WOB are less and the process is more efficient.

3 Estimates for the Efficiency of the AR Method

Let us estimate the efficiency of the AR method for sampling the vector $\mathbf{w}$ with density $p(\mathbf{w}|r)$.

In the case when $p(r) = e^{-b^* r}$ we can bound the function $h(r)$ more precisely:

$$h(r) = 2 - \frac{e^{b^* r}}{e^{b^* R}} \leq 2 - \frac{1}{e^{b^* R}} = H.$$

Now we can use the constant H as a majorant function for the AR algorithm.

The following formula gives us the efficiency of the AR method:

$$Eff_T = \int_0^{2\pi} \int_0^{\pi} p(\mathbf{w}|r) d\theta d\varphi \Bigg/ \int_0^{2\pi} \int_0^{\pi} \frac{sin(\theta)}{4\pi} H d\theta d\varphi$$

The majorant functions (H) and the theoretical estimates (Eff_T) for the AR efficiency in the all cases for $p(r)$ are given in Table 1. Taking in account that

Table 1. The majorant functions and the estimates for the AR efficiency.

$p(r)$	H	Eff_T
$e^{-b^* r}$	$2 - 1/e^{b^* R}$	$(2 - 1/e^{b^* R})^{-1}$
$const$	$1 + b^* R$	$(1 + b^* R)^{-1}$
$e^{b^* r}$	$e^{b^* R}$	$(e^{b^* R})^{-1}$

$0 < \frac{1}{e^{b^* R}} < 1$ and inequalities (15) and (16), for all three choices for the $p(r)$, the following estimate for the efficiency of the AR method is obtained:

$$Eff_T \geq 1/2.$$

4 Numerical Tests

As an example the following boundary value problem was solved using the MC algorithms under consideration:

$$\sum_{i=1}^{3} \left(\frac{\partial^2 u}{\partial x_i^2} + b_i(x) \frac{\partial u}{\partial x_i} \right) + c(x) u = 0 \quad \text{in} \quad \Omega = [0,1]^3,$$

$$u(x_1, x_2, x_3) = e^{a_1 x_1 + a_2 x_2 + a_3 x_3}, \qquad x \in \partial\Omega_\varepsilon.$$

In our tests, we have: $b_1(x) = a_2 a_3 (x_2 - x_3)$, $b_2(x) = a_3 a_1 (x_3 - x_1)$, $b_3(x) = a_1 a_2 (x_1 - x_2)$, and $c(x) = -(a_1^2 + a_2^2 + a_3^2)$, where a_1, a_2, a_3 are the parameters.

It is easy to see that $div\mathbf{b}(x) = 0$. This condition guarantees the possibility to use the local integral representation by Green's function.

A large number of experiments are done that investigate the computational cost of the presented MC algorithms and the efficiency of the AR method for different values of the coefficients $a_i, i = 1, 2, 3$. Some of them that estimate

Table 2. $u(x)$=1.454991, a_1=a_2=a_3=0.25, N=5000, b^*=0.108, $\overline{R}$=0.5

$p(r)$	Eff_T	$\varepsilon = 0.01$		$\varepsilon = 0.05$	
		Eff_P	err	Eff_P	err
e^{-b^*r}	0.949949	0.987592	-0.003216	0.979795	-0.001380
$const$	0.948653	0.987223	0.001937	0.979358	0.000372
e^{b^*r}	0.947312	0.987142	0.003435	0.979248	0.003498

the solution at a point with coordinates (0.5, 0.5, 0.5) for two ε-strips, ε = 0.01 and ε = 0.05, are presented in Table 2. Here, $u(x)$ = 1.454991 is the exact solution; err is the relative error; Eff_T is the value of the theoretical AR efficiency and Eff_P is the AR efficiency from our experiments. We see that the numerical tests for the AR efficiency confirm the theoretical results.

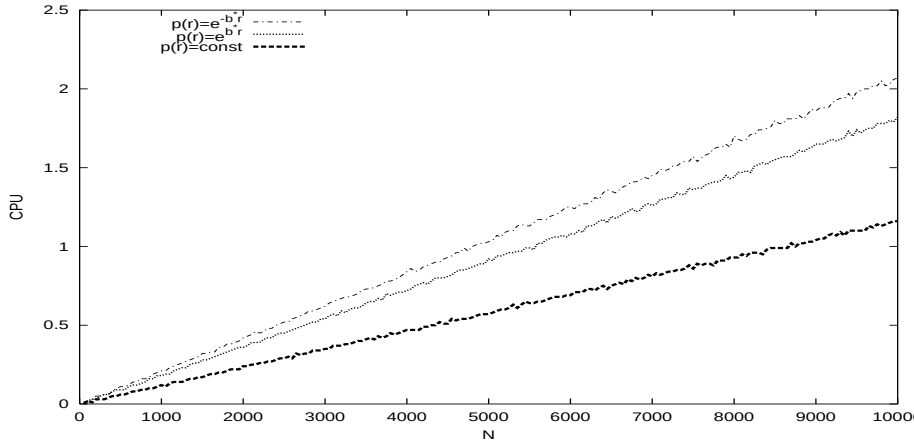

Fig. 1. The CPU times for all algorithms when $\varepsilon = 0.01$, $b^* = 1.732051$.

Figure 1 shows CPU times of the MC algorithms using the three different density functions. In the case, when $p(r) = const.$ the computational cost is less than other two cases for $p(r)$. When the function $p(r) = e^{b^*r}$, the CPU time is less than the case when $p(r) = e^{-b^*r}$. This can be explained with results for the average moves in the WOB that are presented in Table 3. Thus, the numerical results show that it is better to use both constant density and exponential density with positive degree if the parameters of the boundary value problem allow.

In conclusion a new class of grid-free MC algorithms have been studied for solving the elliptic boundary value problem under consideration. The density function $p(\rho)$ which is used in the definition of the Levy's function 6 have be chosen to depend only on the advection. This choice allows the integral transfor-

Table 3. The average number of moves in the WOB. $u(x) = 1.454991$, $\varepsilon = 0.01$

$p(r)$	El_ε		
	$a_i = 0.25$, $b^* = 0.108$	$a_i = 0.5$, $b^* = 0.433$	$a_i = -1$, $b^* = 1.732$
$e^{-b^* r}$	36.319736	36.745987	38.757385
$const$	36.115093	36.178699	36.148346
$e^{b^* r}$	35.952934	35.590324	33.949802

mation kernel be non-negative in the case when deposition is zero. Thus, it has used as a transition density at the Markov chain. An estimate for the efficiency of the applied AR method have been obtained. This estimate has the same rate as the estimate of Ermakov, Nekrutkin and Sipin [6]. The difference is that their estimate is obtained when $p(\rho)$ is taken to be an exponential density with negative degree. Also, it depends on the advection, on the deposition, and on the radius of the maximal ball lying inside the domain Ω. Therefore, we solve the problem in more common case without some limitations as dependence on the deposition and on the radius of the maximal ball.

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