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Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Functional Random Walk on Spheres algorithm for biharmonic equation: optimization and error estimation

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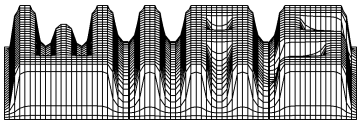
No. 826
Berlin 2003



1991 *Mathematics Subject Classification.* 65C05, 76S05.

Key words and phrases. Random Walk on Spheres algorithm, global estimators, biharmonic equation, optimization and error estimation, multilinear interpolation.

The support by the European Grants INTAS-99-1501 and INTAS YSF 2001/2-53, the NATO Linkage Grant 978912 and Russian Foundation of the Basic Research (project 02-01-00958) is kindly acknowledged.

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Abstract

The global algorithm of Random Walk on Spheres suggested in [8] is analyzed and a kind of optimization strategy is suggested. The algorithm is applied here to construct a functional version of this method which uses a multilinear interpolation. As an example we have chosen the biharmonic equation governing the bending of a thin elastic plate with the simply supported boundary, however generalizations to other equations can be carried out.

1. Introduction

Let as consider the biharmonic equation governing the bending of a thin elastic plate

$$\Delta^2 u(x) = f(x), \quad x \in D \subset R^2. \tag{1.1}$$

Here $u(x)$ is the normal displacement of the plate at a point x, $f(x)$ is the intensity of normal load. Domain D is not supposed to be bounded however it is assumed that the domain D is bounded in one direction, i.e., it can be situated between two parallel lines (see [8]).

We assume that the plate edge is simply supported:

$$u\Big|_\Gamma = 0, \quad \Delta u\Big|_\Gamma = 0, \tag{1.2}$$

where Γ is the boundary of the domain D.

The problem is to approximate the solution of the problem (1.1)-(1.2) on some bounded subdomain $\tilde{D} \subset D$ in the whole, i.e., to find a numerical approximation of the solution for an arbitrary set of points in $\tilde{D}$, and then construct an interpolation. To estimate the solution in a set of points we use the global Walk on Spheres algorithm [8].

A possible way of construction of the solution as a function on the whole domain is the following [6, 7, 10, 11, 13]. Take a Monte Carlo estimator ζ (biased or unbiased) for the solution $u(x)$ in an arbitrary fixed point x. We construct a uniform rectangular grid with a mesh size h on the domain $\tilde{D}$

$$\left\{x^{(i)}\right\}_{i=1}^{M} \subset \tilde{D}$$

and use the Monte Carlo algorithm to evaluate the values of the solution in the grid nodes:

$$u(x^{(i)}) \approx \tilde{u}(x^{(i)}) = \frac{1}{N}\sum_{n=1}^{N} \zeta_n^{(i)}, \tag{1.3}$$

where $\zeta_n^{(i)}$ are independent samples of $\zeta^{(i)}$ $(n = 1, \ldots, N)$, $\zeta^{(i)}$ is the random estimator for $u(x^{(i)})$. To calculate u, an interpolation procedure which uses the obtained values at the grid nodes $\tilde{u}(x^{(i)})$ can be then applied.

We use the multilinear interpolation in the form

$$u(x) \approx L_{(M)}\tilde{u}(x) = \sum_{i=1}^{M} \tilde{u}(x^{(i)})\chi_i(x). \tag{1.4}$$

Here

$$\chi_i(x) = \chi_{(i_1,\ldots,i_d)}(x_1,\ldots,x_d) = \chi\left(\frac{x_1}{h} - i_1\right)\cdots\chi\left(\frac{x_d}{h} - i_d\right),$$

where $(i_1,\ldots,i_d)$ is the multi-index corresponding to the node $x^{(i)}$ so that $x^{(i)} = (i^{(1)}h,\ldots,i^{(d)}h)$, and

$$\chi(s) = \begin{cases} 1+s, & \text{if} \quad -1 \le s \le 0\,, \\ 1-s, & \text{if} \quad 0 \le s \le 1\,, \\ 0 & \text{else} \end{cases}$$

is a finite piecewise-linear generating function. Implementation of this approximation is simple, and it is possible to estimate the upper bound of the error of the algorithm under study.

We use the following global Monte Carlo algorithm to calculate the values of the solution u of problem (1.1)- (1.2) at the grid nodes $x^{(i)}$ [8]. The solution of problem (1.1)-(1.2) at the grid nodes is represented in the form

$$u(x^{(i)}) = \int_D u_\delta(x^{(i)},y)f(y)\,dy, \tag{1.5}$$

where u_δ is the Green function defined by

$$\Delta^2 u_\delta(x,y) = \delta(x-y), \quad u_\delta\Big|_{x\in\Gamma} = 0, \quad \Delta u_\delta\Big|_{x\in\Gamma} = 0.$$

Let

$$u_\delta(x^{(i)},y) = V(x^{(i)},y) + W(x^{(i)},y), \tag{1.6}$$

where $V(x^{(i)},y) = \frac{|x^{(i)}-y|^2}{8\,\pi}\ln|x^{(i)}-y|$ is the fundamental solution of the biharmonic equation. For $W(x,y)$ we then have the following problem

$$\Delta^2 W(x,y) = 0, \quad W\Big|_{x\in\Gamma} = -V\Big|_{x\in\Gamma}, \quad \Delta W\Big|_{x\in\Gamma} = -\Delta V\Big|_{x\in\Gamma}. \tag{1.7}$$

Note that here $y \in D$ is a parameter.

For the problem of type (1.7), namely

$$\Delta^2 v = 0, \quad v\Big|_{\Gamma} = \varphi_1, \quad \Delta v\Big|_{\Gamma} = \varphi_2\ , \tag{1.8}$$

the random estimator can be constructed through a randomized evaluation of the spherical mean value relation [8]:

$$v(y) = N_y^R(v) - \frac{R^2}{4}N_y^R(\Delta v), \quad \Delta v(y) = N_y^R(\Delta v),$$

where N_y^R is the averaging operator over sphere $S(y,R)$ centered at the point y, whose radius equals to R, i.e.,

$$N_y^R(v) = \frac{1}{2\pi R}\int_{S(y,R)} v\,dS. \tag{1.9}$$

This random estimator is associated with the local Walk on Spheres process in the domain D. In order to describe it in more details, we introduce the notation: $\bar{D}$ is the closure of the domain D, $d(x)$ is the distance from the point x to the boundary Γ, Γ_ε is an ε-neighborhood of the boundary Γ, i.e.

$$\Gamma_\varepsilon = \{x \in \bar{D} : d(x) < \varepsilon\}.$$

$\{y_0, y_1, \ldots, y_{L_\varepsilon}\} \subset D$ is the trajectory of Walk on Spheres process starting at the point $y_0 = y$, and $y_{l+1} = y_l + d(y_l)\omega_l, \quad l = 0, 1, \ldots,$ where $\{\omega_l\}$ are mutually independent random unit isotropic vectors, L_ε is a random number of steps the process spends in $D \setminus \Gamma_\varepsilon$ before its first passage of Γ_ε . Thus in the Walk on Spheres process we choose the next point y_{l+1} uniformly on the surface of the maximal sphere with its center at point y_l which lies entirely in the domain $\bar{D}$.

The ε-biased estimator for the solution of the equation (1.8) at a fixed point y reads [8]:

$$\eta_\varepsilon(y) = \varphi_1(y^*) - Q\varphi_2(y^*), \quad Q = \frac{1}{4}\sum_{l=0}^{L_\varepsilon} d^2(y_l), \tag{1.10}$$

where y^* is the point on the boundary Γ closest to $y_{L_\varepsilon} \in \Gamma_\varepsilon$.

In [8] it is shown that the variance $\mathbf{V}\eta_\varepsilon(y)$ is bounded uniformly, as ε tends to zero, and that under some broad smooth-assumptions

$$|v(y) - \mathbf{E}\eta_\varepsilon(y)| \le H\,\varepsilon, \quad y \in D. \tag{1.11}$$

Thus for the solution of problem (1.7) we assume to have an ε-biased random estimator of the type (1.10) and hence we can construct a biased random estimator for $u(x^{(i)})$ using the relations (1.5), (1.6), the symmetry of the Green function and the double randomization method (see for details [8]). This leads us to the global walk on spheres algorithm, so let us present the relevant random estimator. Let $\pi(y)$ be an appropriate distribution density of a point y in the domain D, i.e., $\pi(y) \neq 0$ for all points y for which $f(y) \neq 0$. We denote by $\eta_\varepsilon^{(i)}(y), i = 1, \ldots, M$ the ε-biased random estimators of the type (1.10) for the solution of the problems (1.7) at the point y for all points $x^{(i)}$. Then for the solution of the original problem (1.1) - (1.2) at the grid nodes we obtain the following ε-biased random estimators

$$\zeta_\varepsilon^{(i)} = \frac{f(y)}{\pi(y)}\left(V(x^{(i)}, y) + \eta_\varepsilon^{(i)}(y)\right), \quad i = 1, \ldots, M, \tag{1.12}$$

where the random point y is sampled in D from the density π. We rewrite the estimators (1.12) in the form

$$\zeta_\varepsilon^{(i)} = \frac{f(y)}{\pi(y)}\left(V(x^{(i)}, y) - V(x^{(i)}, y^*) + Q\Delta V(x^{(i)}, y^*)\right), \quad i = 1, \ldots, M. \tag{1.13}$$

To calculate the estimators $\left\{\zeta_\varepsilon^{(i)}\right\}_{i=1}^{M}$ we first sample the point y from the density $\pi(y)$; then simulate the Walk on Spheres process starting in this point y and finishing after its first passage of the ε- neighborhood of the boundary, and calculate estimators by formula (1.13) for each node.

By substituting $\zeta_\varepsilon^{(i)}$ in (1.3), (1.4) we obtain the functional Monte Carlo algorithm with three parameters: M (the number of grid nodes), N (the sample size) and ε. The problem is now: what is the best possible choice of these parameters to minimize the computational cost of algorithm. The exact optimization problem being too complicated, can be treated in a simplified way, by estimating the upper bound of the error and trying to minimize the cost function under some fixed error level.

We consider the error of approximation (1.4) in the metric of continuous function space $\mathbf{C}$, i.e., the quantity

$$\delta = \sup_{x \in \tilde{D}} |u(x) - L_{(M)}\tilde{u}(x)|. \tag{1.14}$$

We use the convergence in probability as probability criterion for the convergence of this error to zero, i.e., we consider the relations of the following type

$$\mathbf{P}\{\delta < T(M, N, \varepsilon)\} > 1 - \theta, \tag{1.15}$$

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

The choice of optimal parameters M, N and ε is based on the upper bounds of the error (1.15). The optimization problem [6] is to minimize the cost function of the algorithm

$$S(M, N, \varepsilon) \quad \text{provided that} \quad T(M, N, \varepsilon) = \alpha, \tag{1.16}$$

where $\alpha > 0$ is some fixed error level.

In section 2 we derive the upper bound of the error of the type (1.15) for the algorithm presented. In section 3 we formulate and solve the optimization problem (1.16). In section 4 we describe the Decentred Random Walk on Spheres which can in many cases essentially improve the efficiency of the algorithm presented. In section 5 we present numerical optimization results for two test problems of the type (1.1)-(1.2) with known exact solutions.

2. The upper bound of the error

According to the triangle inequality the error (1.14) is expanded into three components. They are: (1) the interpolation component, (2) the bias, and (3) the stochastic component:

$$\delta \le \sup_{x \in \tilde{D}} \left| u(x) - L_{(M)}u(x) \right| + \sup_{x \in \tilde{D}} \left| L_{(M)}u(x) - L_{(M)}\hat{u}(x) \right| +$$

$$+ \sup_{x \in \tilde{D}} \left| L_{(M)}\hat{u}(x) - L_{(M)}\tilde{u}(x) \right| = \delta_1 + \delta_2 + \delta_3. \tag{2.1}$$

Here

$$L_{(M)}u(x) = \sum_{i=1}^{M} u(x^{(i)})\chi_i(x), \quad L_{(M)}\hat{u}(x) = \sum_{i=1}^{M} \mathbf{E}\zeta_\varepsilon^{(i)}\chi_i(x).$$

The first two components of the error in (2.1) are deterministic while the third component is random. The first summand δ_1 is the error of the multilinear interpolation. If $u \in \mathbf{C}^{(2)}(\bar{\tilde{D}})$ then there exists a positive constant H_1 such that [5]

$$\delta_1 \le H_1 M^{-1}. \tag{2.2}$$

The second term in (2.1) corresponds to the bias. For multilinear interpolation the error concentrates at the grid nodes, i.e. the following equality holds [10]

$$\delta_2 \leq \max_{i=1,\ldots,M} |u(x^{(i)}) - \mathbf{E}\zeta_\varepsilon^{(i)}|. \tag{2.3}$$

Here $|u(x^{(i)}) - \mathbf{E}\zeta_\varepsilon^{(i)}|$ is the value of the bias at the i-th node. From (1.11) it can be easily found that there exists a positive constant H_2 such that

$$|u(x^{(i)}) - \mathbf{E}\zeta_\varepsilon^{(i)}| \leq H_2\,\varepsilon. \tag{2.4}$$

The third summand in (2.1) is the stochastic component of the error. As for the bias, this error concentrates at the grid nodes, i.e.,

$$\delta_3 \leq \max_{i=1,\ldots,M} |\mathbf{E}\zeta_\varepsilon^{(i)} - \tilde{u}(x^{(i)})|.$$

Writing the expression for $\tilde{u}(x^{(i)})$ in more details, we obtain

$$\delta_3 \leq \max_{i=1,\ldots,M} \left| \mathbf{E}\zeta_\varepsilon^{(i)} - \frac{1}{N}\sum_{n=1}^{N} \zeta_{\varepsilon,n}^{(i)} \right|. \tag{2.5}$$

Note that the random estimators $\zeta_\varepsilon^{(i)}$ for the problem (1.1)-(1.2) at the grid nodes look very similar to the so-called Dependent Sampling Method [2, 14] because it uses the same trajectories for estimating the solution at all grid nodes. But before using the theory of Dependent Sampling Method, we have to verify that this method satisfies the convergence conditions.

Let us consider a random field $\zeta(x)$ defined on the domain $\tilde{D}$ such that $\zeta(x^{(i)}) = \zeta_\varepsilon^{(i)}$. We denote by $g(x) = \mathbf{E}\zeta(x)$, and introduce the estimator for $g(x)$:

$$g_N(x) = \frac{1}{N}\sum_{n=1}^{N} \zeta_n(x),$$

where $\zeta_n(x)$ are independent samples of random field $\zeta(x)$.

We introduce also the sequence of random fields

$$\xi_N(x) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} \tilde{\zeta}_n(x) = \sqrt{N}\,(g_N(x) - g(x))\,,$$

where $\tilde{\zeta}(x) = \zeta(x) - \mathbf{E}\zeta(x)$.

Lemma 1 [14]

Let us assume that the following conditions are satisfied:

a) there exists a positive constant H_V such that

$$\mathbf{V}\tilde{\zeta}(x) < H_V, \quad x \in \tilde{D};$$

b) samples of the random field $\tilde{\zeta}(x)$ are continuously differentiable on $\tilde{D}$ and

$$\mathbf{E}\left|\frac{\partial\tilde{\zeta}(x)}{\partial x_i}\right|^p < C, \quad i=1,\ldots,d, \quad p \geq \max(2, d+\beta), \quad \beta > 0 \tag{2.6}$$

for any $x \in \tilde{D}$ (here d is the dimension of the field).

Then the sequence of random fields $\{\xi_N\}$ weakly converges to a continuous in probability Gaussian random field ξ_0 with zero mean and covariations

$$\mathbf{E}\xi_0(x)\xi_0(y) = \mathbf{E}\tilde{\zeta}(x)\tilde{\zeta}(y), \quad x, y \in \tilde{D}.$$

Moreover, the deviation of the estimator $g_N(x)$ from $g(x)$ has the order of magnitude $N^{-1/2}$ in probability, i.e.,

$$\mathbf{P}\left\{\sup_{x\in\tilde{D}}|g_N(x)-g(x)| \leq C_0\, N^{-1/2}\right\} \to \mathbf{P}\left\{\sup_{x\in\tilde{D}}|\xi_0(x)| \leq C_0\right\} \quad as \quad N\to\infty. \tag{2.7}$$

Convergence (2.7) implies that for any $\theta > 0$ there exists a positive constant $H_3(\theta)$ and an integer number $\hat{N}(\theta)$ such that the following inequality holds

$$\mathbf{P}\left\{\sup_{x\in\tilde{D}}\left|\mathbf{E}\zeta(x) - \frac{1}{N}\sum_{n=1}^{N}\zeta_n(x)\right| \leq H_3(\theta)\, N^{-1/2}\right\} > 1-\theta \tag{2.8}$$

for any $N > \hat{N}(\theta)$.

Now we have to verify that the conditions a) and b) of this Lemma are satisfied for the corresponding random field $\zeta(x)$. From (1.13) we derive that

$$\zeta(x) = \frac{f(y)}{\pi(y)}\left(V(x,y) - V(x,y^*) + Q\Delta V(x,y^*)\right), \tag{2.9}$$

where $V(x,y)$ is the fundamental solution of biharmonic equation

$$V(x,y) = \frac{|x-y|^2}{8\,\pi}\,\ln|x-y|, \quad \Delta V(x,y) = \frac{\ln|x-y|+1}{2\,\pi}.$$

It is easy to show that the variance boundedness of randomized estimators $\zeta_\varepsilon^{(i)}$ follows from the variance boundedness of the estimators of the type (1.10), and from finiteness of the integral $\int\limits_D \frac{f^2(y)}{\pi(y)}\,dy$. But the variance boundedness of randomized estimators $\zeta_\varepsilon^{(i)}$ implies that the condition a) of the Lemma 1 is satisfied.

Further note that when verifying the conditions b), we can restrict ourselves to the domain $\tilde{D}\setminus\Gamma_\varepsilon$ because we can suppose that all the grid nodes lie in $\tilde{D}\setminus\Gamma_\varepsilon$. Since $y^* \in \Gamma$, the second and third summands in (2.9) have no singularities on the domain $\tilde{D}\setminus\Gamma_\varepsilon$ ($|x-y^*| \geq \varepsilon$). Thus we have to investigate only the first summand but the function $V(x,y)$ is continuously differentiable with respect to x. Therefore, samples of the random field $\tilde{\zeta}(x)$ are continuously differentiable on $\tilde{D}\setminus\Gamma_\varepsilon$. The condition (2.6) follows from this fact and the boundedness of domain $\tilde{D}$. Consequently, the condition b) of the Lemma 1 is satisfied, too. Thus we have by Lemma 1 that for the random field $\zeta(x)$ the inequality

(2.8) holds. To obtain the upper bound for the stochastic component of the error δ_3 of the type (1.15) we can use the following inequality

$$\mathbf{P}\left\{\max_{i=1,\ldots,M}\left|\mathbf{E}\zeta_{\varepsilon}^{(i)}-\frac{1}{N}\sum_{n=1}^{N}\zeta_{\varepsilon,n}^{(i)}\right|\leq H_3N^{-1/2}\right\}\geq\mathbf{P}\left\{\sup_{x\in\tilde{D}}\left|\mathbf{E}\zeta(x)-\frac{1}{N}\sum_{n=1}^{N}\zeta_n(x)\right|\leq H_3N^{-1/2}\right\}. \tag{2.10}$$

Now combining (2.1)-(2.5), (2.10), (2.8) we obtain the following theorem about the upper error bound of the algorithm.

Theorem 1 *Assume that the following conditions are satisfied*

a) there exists a constant C_1 *such that* $\int\limits_D \frac{f^2(y)}{\pi(y)}\,dy < C_1$,

b) all grid nodes $x^{(i)}$ *lie in* $\tilde{D}\setminus\Gamma_\varepsilon$.

Then for any $\theta>0$ *there exist some positive constants* H_1, H_2, $H_3(\theta)$ *and an integer number* $\hat{N}(\theta)$ *such that the following inequality holds*

$$\mathbf{P}\left\{\delta\leq H_1\,M^{-1}+H_2\,\varepsilon+H_3N^{-1/2}\right\}>1-\theta, \tag{2.11}$$

for any $N>\hat{N}(\theta)$

3. Optimization problem

Thus we have obtained the upper bound of the error for the functional algorithm, and we can formulate the optimization problems of the type

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

where $S(M,N,\varepsilon)$ is the cost function and $T(M,N,\varepsilon)$ is the upper bound of the error from (2.11).

The cost function of the algorithm has the form

$$S(M,N,\varepsilon)=N\,(t_1\,\mathbf{E}L(\varepsilon)+t_2\,M)=S_1+S_2, \tag{3.1}$$

where $\mathbf{E}L(\varepsilon)$ is the average number of spheres per one trajectory and its order of magnitude is $|\ln\varepsilon|$ (e.g., see [1, 8]), t_1 is the average computer time per one step in the Walk on Spheres process, t_2 is the computer time of calculation of functions per one grid node (see (1.13)).

On the other hand let us fix the upper bound of the error by some error level α :

$$\frac{H_1}{M}+H_2\varepsilon+\frac{H_3}{\sqrt{N}}=\alpha. \tag{3.2}$$

Treating the optimization in the sense of order of magnitude, we obtain from (3.2) that

$$\varepsilon=O(\alpha),\quad M=O\left(\frac{1}{\alpha}\right),\quad\text{as}\quad\alpha\to0.$$

Therefore, $|\ln\varepsilon| = O(|\ln\alpha|)$ and the first component S_1 of the cost function is more lesser than the second component S_2 as $\alpha \to 0$:

$$t_1\,\mathbf{E}L(\varepsilon) << t_2\,M, \quad \text{as} \quad \alpha \to 0.$$

So it is reasonable to neglect the first component S_1 of the cost function and to obtain the following optimization problem which is simpler:

$$\min_{M,N,\varepsilon} S_2(M,N,\varepsilon) \quad \text{provided that}$$

$$\frac{H_1}{M} + H_2\varepsilon + \frac{H_3}{\sqrt{N}} = \alpha, \tag{3.3}$$

where

$$S_2(M,N,\varepsilon) = t_2\,N\,M. \tag{3.4}$$

First we fix ε and find optimal values $M_{opt}(\varepsilon)$ and $N_{opt}(\varepsilon)$. Find N from (3.3) and substitute it in (3.4):

$$S_2 = \frac{t_2 H_3^2 M}{(\alpha - H_2\varepsilon - H_1/M)^2}.$$

Taking the derivative of this expression with respect to M and set it equal to zero we find

$$M_{opt}(\varepsilon) = \frac{3\,H_1}{\alpha - H_2\varepsilon}, \quad N_{opt}(\varepsilon) = \frac{9\,H_3^2}{4(\alpha - H_2\varepsilon)^2}. \tag{3.5}$$

Further we have to minimize the cost function (3.1) on ε. We substitute (3.5) to (3.1):

$$S_{opt}(\varepsilon) = \frac{C_1|\ln\varepsilon|}{(\alpha - H_2\varepsilon)^2} + \frac{C_2}{(\alpha - H_2\varepsilon)^3} = S_1(\varepsilon) + S_2(\varepsilon). \tag{3.6}$$

Here we have to consider only the first component $S_1(\varepsilon)$ because the second component $S_2(\varepsilon)$ decreases monotone as $\varepsilon \to 0$. Taking the derivative of $S_1(\varepsilon)$ with respect to ε and setting it equal to zero we find the following equation

$$\alpha - H_2\varepsilon = 2H_2\varepsilon|\ln\varepsilon|. \tag{3.7}$$

We denote by ε_{opt} the solution of equation (3.7). It gives the minimum to the function $S_1(\varepsilon)$. Substituting (3.7) to (3.6), we obtain the following function

$$S^*_{opt}(\varepsilon_{opt}) = \frac{C_1}{4\,H_2^2\varepsilon_{opt}^2|\ln\varepsilon_{opt}|} + \frac{C_2}{8\,H_2^3\varepsilon_{opt}^3|\ln\varepsilon_{opt}|^3}\ . \tag{3.8}$$

We cannot solve the equation (3.7) analytically but we can find the asymptotically optimal value ε. It is obvious from the equation (3.7) that the following inequality is satisfied for its solution

$$\varepsilon_{opt}|\ln\varepsilon_{opt}| < \frac{\alpha}{2\,H_2}.$$

Therefore

$$|\ln\varepsilon_{opt}| > |\ln\alpha|$$

asymptotically as $\alpha \to 0$. Then

$$\varepsilon_{opt} < \frac{\alpha}{2\,H_2|\ln\alpha|} = \varepsilon_0 \quad \text{as} \quad \alpha \to 0. \tag{3.9}$$

It is easy to verify that the function S^*_{opt} from (3.8) decreases on the interval $0 < \varepsilon < e^{-1}$. Hence if we replace ε_{opt} by the larger value ε_0, the value $S^*_{opt}(\varepsilon_{opt})$ decreases:

$$S^*_{opt}(\varepsilon_{opt}) > \frac{C_1|\ln\alpha|}{\alpha^2} + \frac{C_2}{\alpha^3} = S_3(\alpha).$$

On the other hand if we substitute a nonoptimal value ε_0 in the cost function $S_{opt}(\varepsilon)$ from (3.6) then its value becomes larger than that for optimal ε_{opt} :

$$S_{opt}(\varepsilon_{opt}) = S^*_{opt}(\varepsilon_{opt}) < S_{opt}(\varepsilon_0) = \frac{C_1|\ln\alpha|}{\alpha^2}\left(1 - \frac{1}{2|\ln\alpha|}\right)^2 + \frac{C_2}{\alpha^3}\left(1 - \frac{1}{2|\ln\alpha|}\right)^3 = S_4(\alpha).$$

$S_3(\alpha)$ is asymptotically close to $S_4(\alpha)$ as $\alpha \to 0$. Consequently the value ε_0 is asymptotically optimal and

$$M_{opt}(\varepsilon_0) = \frac{3\,H_1}{\alpha\left(1 - \frac{1}{2|\ln\alpha|}\right)}, \quad N_{opt}(\varepsilon_0) = \frac{9\,H_3^2}{4\alpha^2\left(1 - \frac{1}{2|\ln\alpha|}\right)}. \tag{3.10}$$

Thus asymptotically optimal value of the cost function has the following order on α :

$$S_{opt} = O(\alpha^{-3}).$$

4. Decentred Random Walk on Spheres

There is a different version of the Walk on Spheres method which can in many cases essentially improve the efficiency. In [9] we have applied the Decentred Random Walk on Spheres (DRWS) method for solving the biharmonic equation of the type (1.8) which is based on the spherical mean value relation written not for the center of the circle $S(x_0, R)$ like (1.9) but for an arbitrary point in the disk: $x \in K(x_0, R)$ ([9]):

$$\begin{aligned} u(x) &= \frac{R^2 - r^2}{2\pi R} \int\limits_{S(x_0,R)} \frac{u(y)dS_y}{|x-y|^2} \\ &+ \frac{R^2 - r^2}{4\pi R} \int\limits_{S(x_0,R)} \left[\frac{R\sin\alpha}{|x-x_0|}\mathrm{arctg}\left\{\frac{|x-x_0|\sin\alpha}{R - |x-x_0|\cos\alpha}\right\}\right. \\ &- \left.\frac{1}{2} - \frac{R\cos\alpha}{2|x-x_0|}\ln\frac{|x-y|^2}{R^2}\right]\Delta u(y)dS_y\ , \end{aligned} \tag{4.1}$$

$$\Delta u(x) = \frac{R^2 - r^2}{2\pi R} \int\limits_{S(x_0,R)} \frac{\Delta u(y)dS_y}{|x-y|^2}\ .$$

Here $r = |x - x_0|$ is the distance from x to the circle's center x_0, and α is the angle between the vectors $x - x_0$ and $y - x_0$.

Note that the first integral in (4.1) is exactly the Poisson formula for the Laplace equation. It is not difficult to find out that the function

$$p(y;x) = \frac{R^2 - |x - x_0|^2}{2\pi R} \cdot \frac{1}{|x - y|^2}$$

is a probability density function of the variable $y \in S(x_0, R)$, for all $x \in K(x_0, R)$. This follows from the representation of the solution $u = 1$ to the Dirichlet problem for the Laplace equation $\Delta u(x) = 0,\ u(x)|_{x \in S(x_0,R)} = 1$ through the Poisson integral.

To sample the point y on the circle $S(x_0, R)$ according to the density $p(y;x)$, the following method can be used [9]:

1. Sample a random direction in the "upper semisphere" $\omega = (\omega_1, \omega_2) = (\cos(\psi), \sin(\psi))$, where ψ is uniformly distributed between 0 and π.

2. Find $y = y_1$ on the circle $S(x_0, R)$ as the intersection point of $S(x_0, R)$ and the ray $x + \omega\,|x - y|$, and find also $y = y_2$ as the intersection point of $S(x_0, R)$ with the ray $x - \omega\,|x - y|$.

3. Let $a_1 = |x - y_1|$, and $a_2 = |x - y_2|$. Then with probability $a_1/(a_1 + a_2)$ take $y = y_2$, and with probability $a_2/(a_1 + a_2)$ take $y = y_1$.

The algorithm has two remarkable properties: (1) the simulation algorithm is the same in arbitrary dimensions, and (2) the closer the point x to the boundary $S(x_0, R)$, the larger is the probability that the random point y is sampled on a part of $S(x_0, R)$ closest to x.

Now we can give the definition of the DRWS process $\{Y_1 = x, Y_2, \ldots, Y_m\}$ starting from an arbitrary point $Y_1 = x \in K(x_{01}, R_1)$: let Y_2 be a random point sampled on $S(x_{01}, R_1)$ as described in the above algorithm. As the second disc, choose one of the discs satisfying the condition $K(x_{02}, R_2) \subset G$ and $Y_2 \in K(x_{02}, R_2)$. Then on $S(x_{02}, R_2)$ we sample the point Y_3 as described above for Y_2, etc, till the last point Y_m hits the ε-boundary. Thus starting from the point $x = Y_1$, we then have a sequence of random points $\{Y_2, \ldots, Y_m\}$ which are sampled on the corresponding circles $S(x_{02}, R_2), \ldots, S(x_{0m}, R_m)$.

The random estimator has a form similar to (1.10):

$$\xi_1(x) = g_0(Y_m) - g_1(Y_m) \sum_{k=2}^{m} Q(Y_{k-1}, Y_k)\ .$$

Here

$$Q(Y_{k-1}, Y_k) = \frac{|Y_{k-1} - Y_k|^2}{2} \left[\frac{R_{k-1} \sin(\alpha_k)}{|Y_{k-1} - x_{0k-1}|} \operatorname{arctg} \left\{ \frac{|Y_{k-1} - x_{0k-1}| \sin(\alpha_k)}{R_{k-1} - |Y_{k-1} - x_{0k-1}| \cos(\alpha_k)} \right\} \right.$$
$$\left. -\frac{1}{2} - \frac{R_{k-1} \cos(\alpha_k)}{2|Y_{k-1} - x_{0k-1}|} \ln \frac{|Y_{k-1} - Y_k|^2}{R_{k-1}^2} \right],$$

α_k is the angle between the vectors $Y_{k-1} - x_{0k-1}$ and $Y_k - x_{0k-1}$.

The DRWS process is much faster than the standard walk on spheres process: the mean number of steps to reach the ε-boundary behaves like $\ln|\ln(\varepsilon)|$ instead of $|\ln(\varepsilon)|$, see [3, 4].

However the faster convergence to the boundary does not change essentially the conclusion about the choice of optimal parameters, and hence in practice this method can be applied after choosing the optimal parameters as described in the previous section.

5. Numerical experiments

5.1. Test problem for the thin elastic rectangular plate

Numerical experiments were carried out for the problem with known exact solution for the thin elastic rectangular plate [12]

$$\Delta^2 u(x) = f(x), \quad u\Big|_\Gamma = 0, \quad \Delta u\Big|_\Gamma = 0,$$

where $x \in D = [0,a] \times [0,b]$,

$$f(x) = C_0 \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{b}\right).$$

The exact solution of this problem is

$$u(x) = C_0 \frac{a^4 b^4}{\pi^4 (a^2+b^2)^2} \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{b}\right).$$

Here it is supposed that $\tilde{D} = D$.

The calculations were made for $C_0 = 1$, $a = 1$, $b = 1$. The random point y where the trajectories start was sampled uniformly in D.

The calculation results for different error levels α with optimal values of the parameters are given in Table 1. Optimal values of the parameters N_{opt}, M_{opt}, ε_{opt} are determined by the formulas (3.9), (3.10). Here necessary constants H_1, H_2 were calculated by the following formulas

$$H_1 = \frac{\operatorname{mes}\tilde{D}}{8}\left(\sup_{x\in\tilde{D}}\left|\frac{\partial^2 u}{\partial x_1^2}\right| + \sup_{x\in\tilde{D}}\left|\frac{\partial^2 u}{\partial x_2^2}\right| + 2\sup_{x\in\tilde{D}}\left|\frac{\partial^2 u}{\partial x_1 \partial x_2}\right|\right),$$

$$H_2 = \max\left(\sup_{x\in\tilde{D}}\left|\frac{\partial u}{\partial x_1}\right|, \sup_{x\in\tilde{D}}\left|\frac{\partial u}{\partial x_2}\right|\right),$$

and the constant H_3 was estimated from some precomputations.

The value σ was estimated as $\max_{i=1,\dots,M}\sqrt{\frac{\mathbf{V}\zeta^{(i)}}{N}}$, where $\mathbf{V}\zeta^{(i)}$ is the sample variance. Through δ_s, δ_i, δ we denote the stochastic, interpolation and total errors, respectively. The stochastic error δ_s was estimated as maximum of the absolute value of the difference between the exact and approximate solutions over the nodes and so it includes the bias

too. The error of interpolation δ_i was estimated by using the difference between the exact solution and solution interpolated over exact value in grid nodes at 10^6 random points from D. Here the total error δ is the sum of the error of interpolation δ_i and the stochastic error δ_s. t is the computer time used to calculate the approximate solution in grid nodes.

The results presented in Table 1 show that the total error does not exceed the permissible level α.

Table 1: Testing of the optimal parameters.

$\alpha\,10^5$	N_{opt}	$\sqrt{M_{opt}}$	$\varepsilon_{opt}10^7$	$\sigma\,10^5$	$\delta_s\,10^5$	$\delta_i\,10^5$	$\delta\,10^5$	t
5	159720	27	2.52	1.30	2.64	0.80	3.44	138
2.5	634461	38	1.18	0.68	1.56	0.42	1.98	1096
1.25	2837793	55	0.55	0.33	0.75	0.20	0.95	9782

In Table 2 we present results of numerical experiments for the same problem but with various nonoptimal relations between parameters M and N. Since the component $S_2 = t_2\,N\,M$ from (3.1) makes higher contribution to the computational cost in comparison with S_1 we varied M and N provided that $M\,N = const$. In this case the computational cost practically has not changing. These results show that the optimization procedure presented may lead indeed to a higher efficiency since the optimal choice of parameters results in a smaller total error δ than in the case of nonoptimal choice under comparable computational cost t.

Table 2: Nonoptimal parameters.

$\alpha\,10^5$	N	M	ε	$\sigma\,10^5$	$\delta_s\,10^5$	$\delta_i\,10^5$	$\delta\,10^5$	t
5	$N_{opt}/8$	$M_{opt}*8$	ε_{opt}	4.10	5.69	0.10	5.79	144
5	$N_{opt}/4$	$M_{opt}*4$	ε_{opt}	2.80	5.11	0.20	5.31	143
5	$N_{opt}/2$	$M_{opt}*2$	ε_{opt}	1.93	3.36	0.39	3.75	142
5	N_{opt}	M_{opt}	ε_{opt}	1.30	2.64	0.80	3.44	138
5	$N_{opt}*2$	$M_{opt}/2$	ε_{opt}	0.89	2.01	1.57	3.58	142
5	$N_{opt}*4$	$M_{opt}/4$	ε_{opt}	0.59	1.18	3.17	4.35	144
5	$N_{opt}*8$	$M_{opt}/8$	ε_{opt}	0.38	0.61	6.13	6.74	156

5.2. Test problem for the thin elastic strip

Let as consider the problem with known solutions in the form of a double series [12]

$$\Delta^2 u(x) = f(x), \quad u\Big|_\Gamma = 0, \quad \Delta u\Big|_\Gamma = 0, \tag{5.1}$$

where $x \in D = [0,a] \times [0,b]$,

$$f(x) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} a_{ij} \sin\left(\frac{i\pi x_1}{a}\right) \sin\left(\frac{j\pi x_2}{b}\right),$$

$$a_{ij} = \frac{4}{ab} \int_0^a \int_0^b f(x_1, x_2) \sin\left(\frac{i\pi x_1}{a}\right) \sin\left(\frac{j\pi x_2}{b}\right) dx_1\, dx_2.$$

The exact solution of this problem is

$$u(x) = \frac{1}{\pi^4} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{a_{ij}}{\left(\frac{i^2}{a^2} + \frac{j^2}{b^2}\right)^2} \sin\left(\frac{i\pi x_1}{a}\right) \sin\left(\frac{j\pi x_2}{b}\right).$$

It is supposed that $a = 100b$, i.e. D is a thin elastic strip. The intensity of normal load f is assumed to be concentrated in a point x^0 :

$$f(x_1, x_2) = \delta(x_1 - x_1^0)\delta(x_2 - x_2^0). \tag{5.2}$$

The numerical solution of the problem (5.1), (5.2) is constructed on some bounded domain $\tilde{D} \subset D$.

The calculations were made for $a = 100, b = 1, x_1^0 = 50, x_2^0 = 0.5$. $\tilde{D} = [49, 49.2] \times [0.5, 0.7]$. The trajectories start from the point x^0 with probability 1.

The calculation results for different error levels α with optimal values of the parameters are given in Table 3. Here the error of interpolation δ_i (and the total error δ) was estimated by using the difference between the exact solution and solution interpolated over exact value in grid nodes (or over approximate value, respectively) at 10^3 random points from $\tilde{D}$. Other notation in this table are coincident with those of Table 1. The results presented in Table 3 show that the total error does not exceed the permissible level α.

This numerical experiments give evidence that the optimal relation between parameters can be used efficiently for approximating the solution even on a small subdomain of an unbounded domain.

Table 3: Testing of the optimal parameters.

$\alpha\, 10^5$	N_{opt}	$\sqrt{M_{opt}}$	$\varepsilon_{opt} 10^4$	$\sigma\, 10^5$	$\delta_s\, 10^5$	$\delta_i\, 10^5$	$\delta\, 10^5$	t
5	1996507	4	3.15	2.38	1.42	2.21	2.18	21.5
2.5	7930765	5	1.47	1.20	1.15	1.28	2.45	108
1	49178864	8	0.54	0.48	0.02	0.42	0.43	1170
0.5	195705024	11	0.26	0.24	0.26	0.20	0.44	7458

6. Conclusions

We consider the functional algorithm of Monte Carlo method for solution of biharmonic equation in the whole on some domain $\tilde{D}$ which uses the fundamental solution and the Walk on Spheres process. We construct a uniform rectangular grid on the domain $\tilde{D}$, use the global algorithm of Random Walk on Spheres to evaluate the values of the solution in the grid nodes and then construct an interpolation.

We construct the upper error bound depending on a parameters M (the number of the grid nodes), N (the sample size) and ε in the metric of continuous function space $\mathbf{C}$.

We formulate and solve optimization problem which consists in minimization of the cost function provided that the upper error bound equals to a some permissible error level α. It is shown that the asymptotically optimal cost value is of the order $S_{opt} = O(\alpha^{-3})$.

References

[1] Ermakov S.M. and Mikhailov G.A. Statistical modeling. : Nauka, Moscow, 1982 (in Russian).

[2] Frolov S. and Chentzov N.N. About calculation by Monte Carlo method definite integrals depending on a parameter. Journal of Computational Mathematics and Mathematical Physics. 1962. V. 2, N 4, P. 714-717 (in Russian).

[3] Golyandina N.E. Some functional inequalities and investigation of a rate of Markov chains to a boundary. Journal of Computational Mathematics and Mathematical Physics. 1991. V. 31, N 7, P. 1029-1041 (in Russian).

[4] Golyandina N. Monte Carlo solution of boundary problems for the Laplace operator. Mathematical methods in stochastic simulation and experimental design: Proc. 2nd St. Petersburg Workshop on simulation, St. Petersburg, June 18 - 21, 1996. St. Petersburg University Press, P.81 - 86.

[5] Marchuk G.I. and Agoshkov V.I. Introduction to projective grid methods. Nauka, Moscow, 1981 (in Russian).

[6] Mikhailov G.A. Minimization of computational costs of non-analogue Monte Carlo methods. Series of Soviet and East European Mathematics. Vol. 5. Singapore: World Scientific, 1991.

[7] Plotnikov M.Yu. and Shkarupa E.V. Error estimation and optimization in $\mathbf{C}$ - space of Monte Carlo iterative solution of nonlinear integral equation. Monte Carlo Methods and Application. 1998. V. 4, N 1, P. 53-70.

[8] Sabelfeld K.K. Monte Carlo methods in boundary problems. Springer-Verlag, Heidelberg - Berlin - New York, 1991.

[9] Sabelfeld K.K. and Shalimova I.A. Random walk on spheres methods for iterative solution of elasticity problems. Monte Carlo Methods and Applications, 2002, vol.8, N2, 171-200.

[10] Shkarupa E.V. and Voytishek A.V. Optimization of discretely stochastic procedures for globally estimating the solution of an integral equation of the second kind. Russian Journal of Numerical Analysis and Mathematical Modelling. 1997. V. 12, N 6, P. 525-546.

[11] Shkarupa E.V. Error estimation and optimization for the frequency polygon method in the C-metric. Journal of Computational Mathematics and Mathematical Physics. 1998. V. 38, N 4, P. 590-603.

[12] Timoshenko S.P. and Voinovsky- Krieger. Theory of Plates and Shells. McGRAW-HILL Book Company, Inc., New York Toronto London, 1959.

[13] Voytishek A.V. On the errors of discretely stochastic procedures in estimating globally the solution of an integral equation of the second kind // Russian Journal of Numerical Analysis and Mathematical Modelling. 1996. V. 11, N 1, P. 71-92.

[14] Voytishek V. and Prigarin S.M. About functional convergence of estimations and models in Monte Carlo method // Journal of Computational Mathematics and Mathematical Physics. 1992. V. 32, N 10, P. 1641-1651 (in Russian).