The Random Walk on the Boundary Method for Calculating Capacitance

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Abstract

In this paper we present the "random walk on the boundary" method for the rapid solution of integral equations that arise in electrostatics and related areas. This method is a Monte Carlo method based on the construction of a Markov chain that is readily interpreted as a random walk along the boundary over which integration in the integral equation is taken. To illustrate the usefulness of this technique, we apply it to the computation of the capacitance of the unit cube. Obtaining the capacitance of the cube usually requires computing the charge density, and this problem has been used as a benchmark by many in the field for algorithms of this kind. Here, the "random walk on the boundary" method does not require charge density computation, and obtains the capacitance of the cube within a statistical error of 2.7×10^{-7}, the most accurate estimate to date.

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1 Introduction

In this paper we present a new class of stochastic algorithms, those based on the "random walk on the boundary" Markov chain. We use these to consider a stochastic computational approach to a classical problem in electrostatics, the so-called Robin problem: the computation of the charge distribution on the surface of a conductor held at a given potential. This problem and related ones are still topical in many technical applications, and not only in electronics but in computational biophysics of biomolecules as well (see e.g. [1,2]). This paper is thus an introduction to the "random walk on the boundary" Monte Carlo method to a class of problems to which this method has never before been applied. We hope this work will convince others of the efficacy of this stochastic method, and encourage them to apply it to their own problems. It should be clear to the reader that while we focus specifically on problems in electrostatics in this paper, that the "walk on the boundary" method is a power tool for solving a variety of elliptic boundary value problems.

Going all the way back to Maxwell's time, the boundary element method was effectively used to solve the Robin problem and to calculate the capacitance as the surface integral of the computed charge density [3]. The common deterministic approach is to divide the conductor surface into segments, and to use a piecewise polynomial (on segments) approximation to the charge density, with the assumption that the discretized segments are sufficiently small. Next, the linear dependence between the segment potentials and their charges makes it possible to reduce the problem to a system of algebraic equations, which can be solved by an appropriate numerical method. Hence the computation of capacitance finally requires one to sum up all the computed segment charges. The accuracy of this computation can be improved by extrapolating the computed solution to a polynomial in $1/N$, where N is the number of subdivisions [4]. The alternative approach to finding the charge density is to calculate it as an element in the eigenspace of a particular integral operator [5,6].

As far as stochastic computational methods are concerned, it is commonly held that these methods are most efficient when point values or linear functionals of the solution are needed, or when a solution is needed to just a few percent accuracy. Generally, when either a global solution or a high accuracy solution is desired, stochastic approaches are not normally considered appropriate. Recently, it has been found that in computing the capacitance, the diffusion limited reaction rate, and other related properties of arbitrary shaped bodies, stochastic simulation algorithms can be competitive with boundary element and other conventional deterministic computational methods [7]. In many cases, simple Brownian dynamics simulations can be substantially refined, making it possible to use the walk on spheres (WOS) [8] and the Green's

function first passage (GFFP) Monte Carlo methods [9]. Elimination of the WOS bias due to the boundary with GFFP, the simulation-tabulation technique [10], and last passage variants of these Monte Carlo algorithms [11] further extend the capabilities of stochastic computational methods when applied to electrostatics problems. The progress achieved so far stimulated our investigation of the "random walk on the boundary algorithm" [12] as applied to capacitance and charge density calculations. The idea of using this method on these types of problems dates back to [13]. Here, we thoroughly investigate the computational algorithm based on this approach, the conditions of its applicability, the rate of convergence, and compare it to other Monte Carlo and deterministic methods when applied to the model problem of finding the capacitance of the unit cube.

2 Surface Potential and the Ergodic Theorem

Let $G \in \mathbb{R}^3$ be a compact set representing an electrical conductor. Our goal is to calculate C, the capacitance of G, and μ, the charge distribution on its surface, ∂G.

Mathematically, the problem is to compute the integral

$$C = \int_{\partial G} \mu(y)\, d\sigma(y)$$

and the function

$$\mu(y) = -\frac{1}{4\pi}\frac{\partial u}{\partial n}(y)\ , \tag{1}$$

defined on ∂G, provided that u satisfies Laplace equation in the exterior of G

$$\Delta u(x) = 0\ .$$

In addition, we impose the condition that $u \to 0$ as $|x| \to \infty$, and that

$$u(y) = 1,\ y \in \partial G\ .$$

Above, $n(y)$ is the unit normal vector pointing towards the *outside* the domain, G.

We assume that the boundary, ∂G, is sufficiently smooth to guarantee the existence and uniqueness of the exterior Dirichlet problem we have formulated.

It is sufficient, for example, to demand that ∂G be a regular piecewise Lyapunov surface [14]. In this case it is possible to represent u as a single layer potential

$$u(x) = \int\limits_{\partial G} \frac{1}{|x-y'|}\mu(y')d\sigma(y') \ ,$$

with a charge density, μ, that is the unknown. In this case u is commonly called the Robin potential.

To find an equation satisfied by μ, we make use of the well-known jump properties of the Robin potential's normal derivative. Hence, we have (for $x \in \mathbb{R}^3 \backslash G$ and $y \in \partial G$, $|\cos\varphi_{yx}| = |\frac{y-x}{|x-y|} \cdot n(y)| \geq \alpha > 0$)

$$\begin{aligned} \frac{\partial u}{\partial n}(y) &= \lim_{x \to y} (\nabla_x u(x)) \cdot n(y) \\ &= -\int\limits_{\partial G} \frac{\cos\varphi_{yy'}}{|y-y'|^2}\mu(y')d\sigma(y') - 2\pi\mu(y) \ . \end{aligned} \tag{2}$$

From (1) and (2) it follows that

$$\mu(y) = \int\limits_{\partial G} \frac{\cos\varphi_{yy'}}{2\pi|y-y'|^2}\mu(y')d\sigma(y') \ ,$$

or in operator notation

$$\mu = K\mu \ .$$

These equations imply that μ is the eigenfunction of the integral operator, K, corresponding to the maximal eigenvalue, which equals 1 [15].

Suppose that G is convex, then the kernel of the integral operator $k(y,y') = \frac{\cos\varphi_{yy'}}{2\pi|y-y'|^2}$ is non-negative and

$$\int\limits_{\partial G} \frac{\cos\varphi_{yy'}}{2\pi|y-y'|^2}d\sigma(y) = 1 \ .$$

This normalization means that $k(y_{n+1}, y_n) = p(y_n \to y_{n+1})$ can be used as a transition probability density to construct a Markov chain $\{y_n\}_{n=1}^{\infty}$ of points on ∂G. This density function corresponds to a uniform distribution of successive

points, y_{n+1}, in the solid angle with vertex y_n. This is the so-called isotropic "random walk on the boundary" [12] process.

Hence, we can think of $\Omega(y', \varsigma) = \int\limits_{\varsigma} k(y, y') d\sigma(y)$ as a probability measure defined for every open set ς in ∂G that is based on choosing points uniformly in a solid angle with the vertex, y', subtended by ς.

If ∂G is strictly convex, then the angle measure, Ω, and surface measure, σ, are absolutely continuous, meaning that $\Omega(y', \varsigma)$ is strictly positive [16]. It is well known [17] that the weakly singular integral operator, K, is completely continuous. Thus, $\Omega(y', \varsigma)$ is regular and we can apply the ergodic theorem to statistics created using this Markov chain [16].

Suppose now that there are planar segments of the boundary. In this case not every set of non-zero surface area $\sigma(\varsigma)$ has non-zero angle measure $\Omega(y', \varsigma)$ for all points $y' \in \partial G$. However, it can be easily shown that the second iteration, K^2, of the integral operator defines a strictly positive measure $\Omega^{(2)}(y', \varsigma) = \int\limits_{\partial G} \Omega(y, \varsigma) k(y, y') d\sigma(y)$. Thus, we can apply the ergodic theorem in this case as well.

Therefore, by this theorem, there exists a positive stationary distribution, Π_∞, of the Markov chain as defined above. This means that

$$\Pi_\infty(\varsigma) = \int\limits_{\partial G} \Pi_\infty(d\sigma(y'))\ \Omega^{(2)}(y', \varsigma)$$

for every open set $\varsigma \subset \partial G$. This also implies that the distribution is absolutely continuous and its density, π_∞, satisfies the equation

$$\pi_\infty(y) = K^2 \pi_\infty(y)\ .$$

Hence, since $\mu = K\mu = K^2\mu$,

$$\mu = C\pi_\infty \tag{3}$$

for some constant C. This constant must equal the capacitance of G, since π_∞ is a probability density.

Here, we made use of the fact that 1 is a simple eigenvalue of the integral operator K and there is only one eigenfunction corresponding to this eigenvalue [14].

By the ergodic theorem [19,18], for an arbitrary initial distribution, Π_0, and bounded function v,

$$I[v] \equiv \int\limits_{\partial G} v(y)\pi_\infty(y)d\sigma(y) = \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} v(y_n) \ . \tag{4}$$

Note, that we use both the even and odd indexed points of the Markov chain in this sum since by (3) $\pi_\infty = K\pi_\infty$.

3 A Monte Carlo Estimator for Computing Capacitance

Consider the Robin potential, u, inside G. The boundary conditions state that the Robin potential is constant and equal to one in G. The interpretation of this hearkens back to elementary physics where one learns that inside a conductor the electrical potential is constant. Thus we have

$$\int\limits_{\partial G} \frac{1}{|x-y'|}\mu(y')d\sigma(y') = 1 \ , \tag{5}$$

for any point $x \in G$. Therefore, we may fix $x \in G$ and set $v(y) = \dfrac{1}{|x-y|}$.

Together, the relations (3), (4), (5) result in the following formula (see [12])

$$C = \left(\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} v(y_n)\right)^{-1} \ , \tag{6}$$

which will be used to calculate the capacitance.

To estimate the computational error, we use a Markov chain version of the central limit theorem [18,19]. It states that $\dfrac{1}{N}\sum\limits_{n=1}^{N} v(y_n)$ tends to a normally distributed random variable with mean $I[v]$ and variance $\sigma^2 N^{-1}$. Here,

$$\sigma^2 = \lim_{N\to\infty} \int\limits_{\partial G} \pi_\infty \left[\frac{1}{\sqrt{N}}\sum_{n=1}^{N} \left(v(y_n) - I[v]\right)\right]^2 \ .$$

This means that the error of our computational algorithm is of the statistical nature. Hence, for a given accuracy ε, the cost of computations is of order $\sigma^2\varepsilon^{-2}$.

To evaluate σ^2, we use the method of batch means [20] with the number of batches, $k+1$, equal to $\sqrt{N}+1$ and the batch size, m, equal to $\sqrt{N}$. Thus we have

$$\sigma^2 = \lim_{m\to\infty,\, k\to\infty} \frac{m}{k} \sum_{i=0}^{k} \left(\frac{1}{m} S_i - \frac{1}{N} S \right)^2 ,$$

where $S_i = \sum_{j=mi+1}^{m(i+1)} v(y_j),\ S = \sum_{i=0}^{k} S_i$.

Note, that the algorithm based on (6) provides a method to obtain the value of the capacitance without explicitly calculating the density, μ.

4 Computing Charge Density

To calculate the charge distribution, we use relations (3) and (4) and construct Monte Carlo estimators for iterations either of the integral operator K or its adjoint. These estimators are based on a "random walk on the boundary" process that is not necessarily isotropic. Let $p(y_n \to y_{n+1})$ be the transition probability density of this Markov chain, $\{y_n, n = 0, 1, \ldots\}$. Then, for some integrable functions $f \in L(\partial G)$ and $h \in L^*(\partial G)$ the direct and adjoint estimators, respectively, are defined as [12]

$$(h, K^n f) = \mathbb{E} Q_n h(y_n) = \mathbb{E} Q_n^* f(y_n) \ .$$

Here

$$Q_0 = \frac{f(y_0)}{p_0(y_0)} \ , \quad Q_{n+1} = Q_n \frac{k(y_{n+1}, y_n)}{p(y_n \to y_{n+1})} \ ,$$

and

$$Q_0^* = \frac{h(y_0)}{p_0(y_0)} \ , \quad Q_{n+1}^* = Q_n^* \frac{k(y_n, y_{n+1})}{p(y_n \to y_{n+1})} \ .$$

Therefore, since we are integrating an absolutely convergent series, we have

$$(h, \mu) = C(h, \pi_\infty) = \lim_{N\to\infty} \frac{C}{N} \sum_{n=1}^{N} (h, K^n \pi_0) \ . \tag{7}$$

It is clear that to compute the density, $\mu(y)$, at some point, $y \in \partial G$, we have to set $h(y_0) = \delta(y - y_0)$. Note, however, that this last equality is valid

only for bounded functions, h. To overcome this, we introduce a partition, $\varsigma_j, j = 1, \ldots, m$, on the boundary surface: $\partial G = \bigcup_{j=1}^{m} \varsigma_j$, and use a piecewise constant approximation for μ. Thus, we reduce the problem to the estimation of a finite number of cell values, or in other words, to a finite number of functionals (7) with different weight functions $h_j(y) = \chi[\varsigma_j](y)/\sigma(\varsigma_j)$. Here $\chi[\cdot]$ is the indicator function.

Hence, it is possible to use a direct estimator, and set $p_0 = f = \pi_0$. From this it follows that for convex G all weights, Q_n, are equal to 1 and so

$$\mu(y) \approx \lim_{N\to\infty} \frac{N_j C}{N\sigma(\varsigma_j)} \quad \text{for} \quad y \in \varsigma_j \ , \tag{8}$$

where N_j is the number of Markov chain points that hit the cell ς_j (see [12]).

We thus arrive at an algorithm that makes it possible to calculate both the capacitance and the charge distribution simultaneously. Initially, we randomly choose a point y_0 on ∂G with probability density π_0. One of the possible choices for such a density is to set $\pi_0(y) = \dfrac{\cos\varphi_{yx}}{2\pi|y-x|^2}$ for some x inside the domain G. This means that y_0 is distributed isotropically within the solid angle with vertex x. Next, we simulate a long Markov chain of points using isotropic "random walk on the boundary," and calculate C^{-1} using (6), and the numbers, N_j, with the methods described above. Finally, using (8) we obtain an approximation to the charge distribution.

5 Computational Results for the Unit Cube

To illustrate the computational technique described, we calculate the capacitance of the unit cube and the charge density on its surface. This problem has no analytic solution, and has long been regarded as a benchmark in the electrostatic theory [3]. Different computational methods were used to solve it: boundary element [21,23,4], finite-difference [22], and stochastic algorithms [24,9,7] as well. The results (in units of $4\pi\epsilon_0$) and their published errors (in different senses) are given in Table 1. The most accurate value obtained so far was due to Read [4]. He used the (deterministic) boundary element method with extrapolation, as was described in the introduction to this paper.

Our result is 0.6606780, with a statistical error (two standard deviations) of 2.7×10^{-7}. This was obtained by using the estimator (6) with $N = 10^{12}$. It is essential to note that to compute the result to the statistical accuracy of 5.4×10^{-5} it took only 30 seconds on an ordinary desktop computer. The same

Table 1
Values for the Capacitance of the Unit Cube

Reitan-Higgins (1951)	0.6555
Greenspan-Silverman (1965)	0.661
Goto et.al. (1992)	$0.6606747 \pm 5 \times 10^{-7}$
Zhou et.al. (1994)	$0.6632 \pm 3 \times 10^{-4}$
Given et.al. (1997)	$0.660675 \pm 1 \times 10^{-5}$
Read (1998)	$0.6606785 \pm 6 \times 10^{-7}$
Hwang-Mascagni (2003)	$0.660683 \pm 5 \times 10^{-6}$
our result	$0.6606780 \pm 2.7 \times 10^{-7}$

computations performed on a k-node cluster with k independent streams of pseudorandom numbers (e. g. from the SPRNG library [25]) would decrease the computational time by factor $1/k$. Also we found out that the ergodic walk on boundary algorithm is the most efficient Monte Carlo method for this problem. It has the smallest variance, the smallest computational complexity, and there is no bias in the estimate.

It essential to note that when computing only the capacitance via the "walk on the boundary algorithm," there is no need to partition the domain surface. However, when also evaluating the charge density, we are compelled to introduce a partition for the purpose of producing a histogram of the computed charge density. It is well known that the charge distribution is singular along discontinuous edges on the surface. For an edge formed at an obtuse angle, θ, the dependence of the density, μ, on the distance, r, from the edge is given by [26] $\mu = \text{const } r^{-\alpha}$, where $\alpha = 1 - \pi/\theta$. For the edge of the cube $\theta = 3\pi/2$, so α is equal to $-1/3$ in this case. To take this singularity into account, we introduce a nonuniform grid on every face of the cube. This is chosen in such a way that every segment has approximately the same total charge. Divisions with M elements on every face were considered, where we took M to be equal to $100^2, 200^2$ and 1000^2. The results show a linear dependence of the logarithm of charge density on the logarithm of the distance to the edge of the cube, with a slope predicted by the theory (see Fig.1). Approximately linear log-log dependence remains valid when we consider the density versus the distance to a vertex along the diagonal line of the cube's face (Fig.2). The computed charge density distribution on the cube's surface is shown in Fig.3.

6 Directions for future research

In this paper we described an application of the ergodic random "walk on the boundary algorithm" for solving elliptic boundary value problems arising from electrostatics, specifically for computing the capacitance of and the charge density on a conducting body. The ergodic random "walk on the boundary" algorithm proved to be extremely efficient in this case. It was used to produce the most accurate calculation known to date for the capacitance of the unit cube. Note, however, that this method is limited to the case of convex conductors. So one of the tasks for future research is to investigate the possibility of and conditions for applying this algorithm to electrostatic (elliptic) problems where the domain may not be convex. This will be particularly important in biophysical calculations where the domain will be the union of spherical atomic surfaces.

It is clear that some of the computational algorithms mentioned here may be more efficient in some special cases, so it is essential to compare these methods, and to propose "rules of thumb" for their use across a broad range of problems. For example, it seems that the backward random walk method is the most appropriate method to calculate point values of the charge distribution. We plan to undertake some model computations comparing all the known algorithms in this context in order to obtain empirical performance data for making such recommendations.

Acknowledgements

The second author (N. A. Simonov) acknowledges the kind hospitality of the School of Computational Science and Information Technology of the Florida State University (FSU), and the support of the FSU College of Arts and Sciences and FSU's Office of Research. In addition, the authors would also like to thank Dr. Ian McKeague for his useful discussions.

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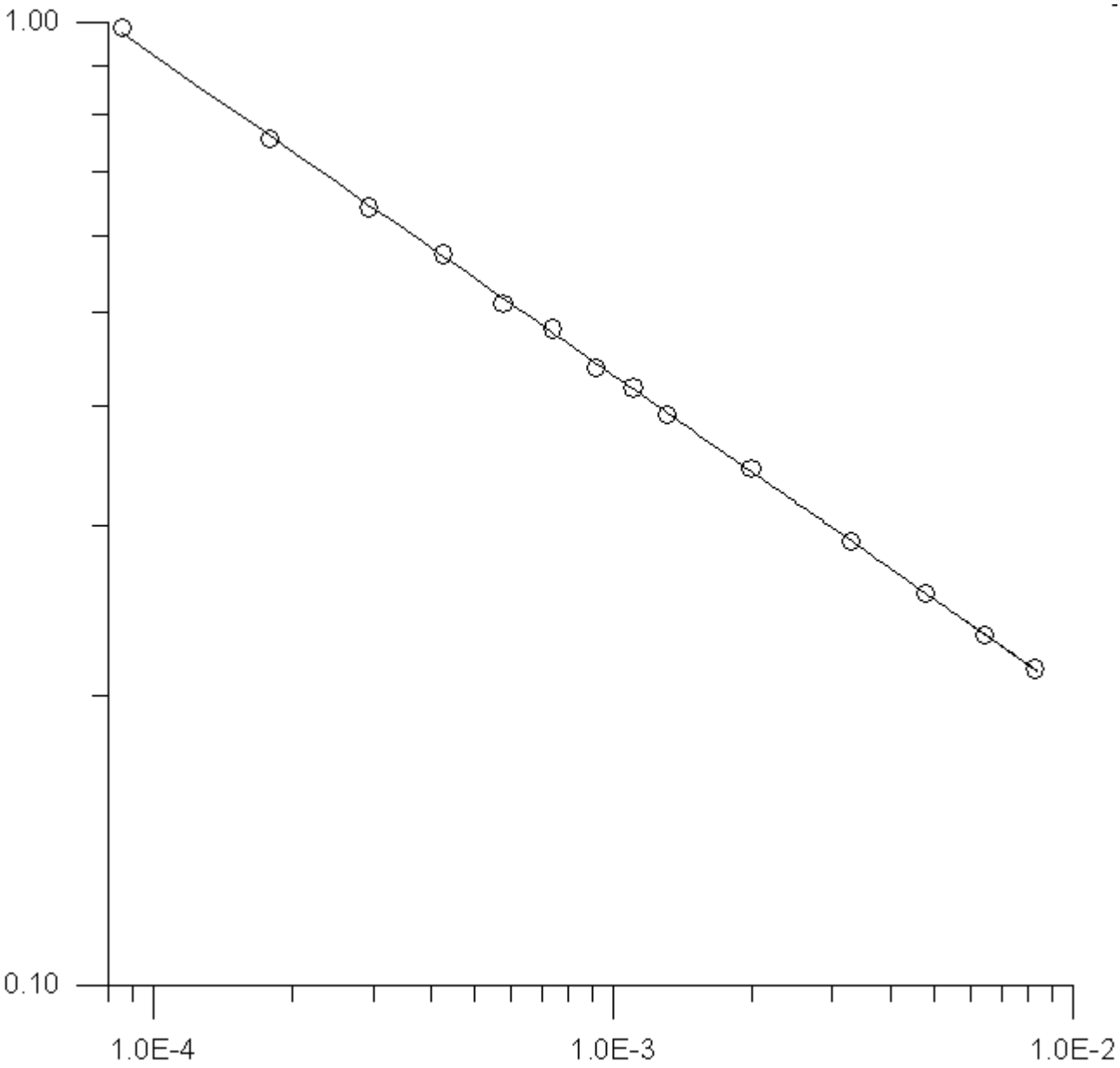

Fig. 1. Log-log plot of charge density versus distance to the edge for the points lying in the middle of the cube's face. Linear regression $\ln \mu = -1.366 - 0.333 \ln r$ (theory gives value $-1/3$ for the second coefficient in the case of the dihedral angle formed by two infinite planes).

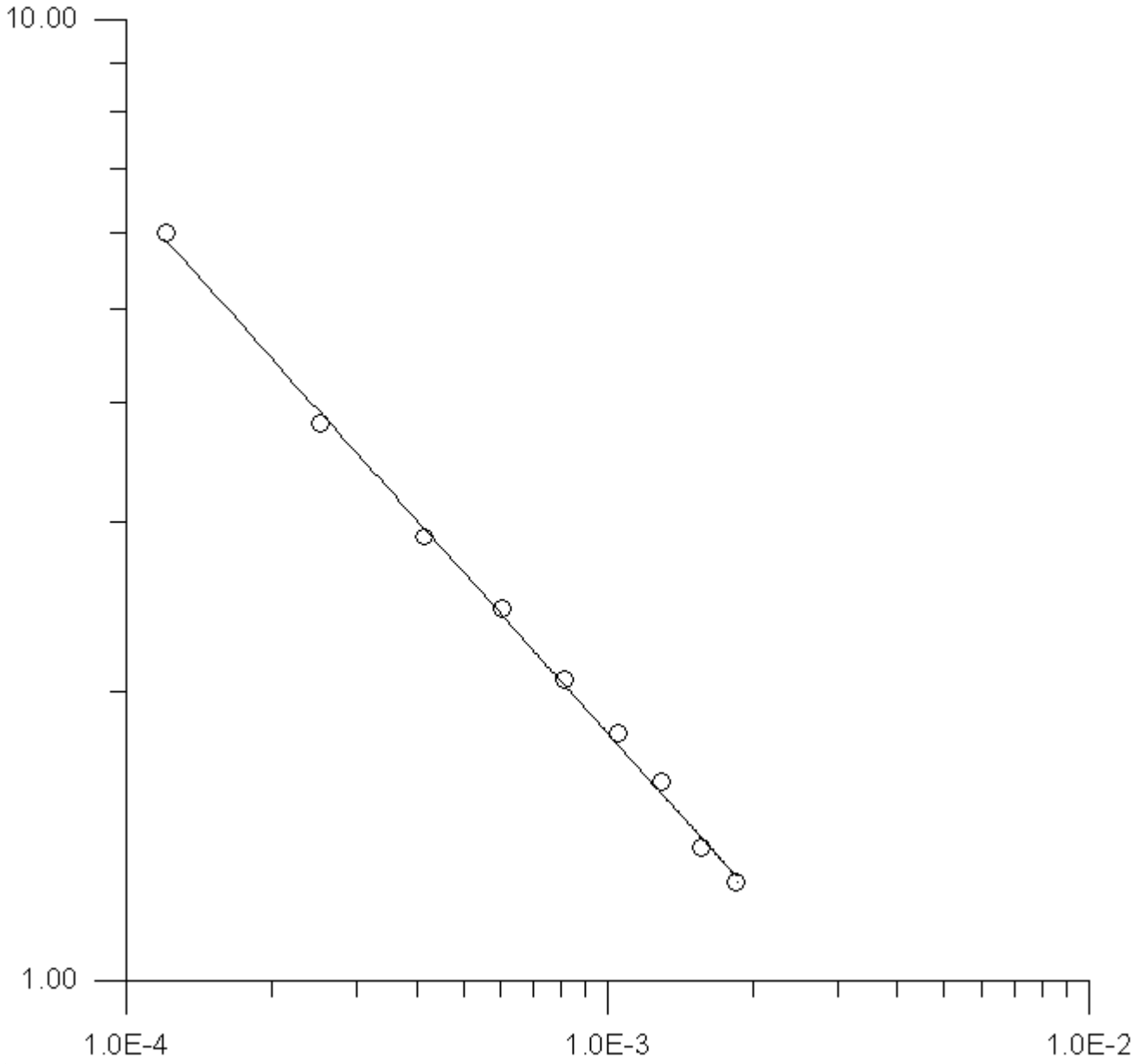

Fig. 2. Log-log plot of charge density versus distance to the cube's vertex along the diagonal. Linear regression $\ln \mu = -1.415 - 0.558 \ln r$.

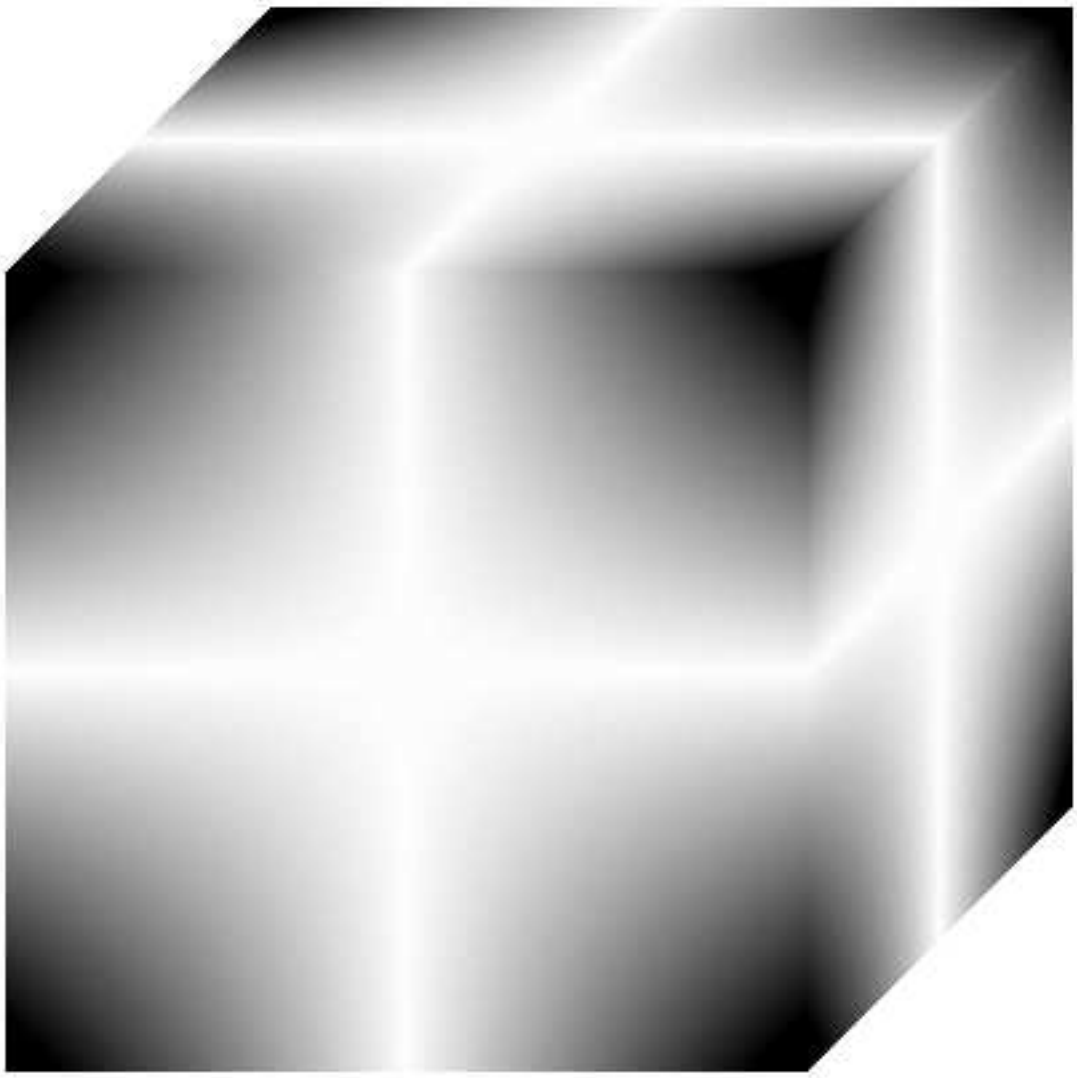

Fig. 3. Charge density distribution on the surface of the unit cube.