

A Monte Carlo Method for Poisson's Equation*

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This investigation presents an analysis of a Monte Carlo method for estimating local solutions to the Dirichlet problem for Poisson's equation. The probabilistic algorithm consists of a modified "walk on spheres" that includes the effects from internal sources as part of the random process. A new derivation of the asymptotic expressions for the rate of convergence and average runtime of the algorithm is presented. These estimates are used to compare the Monte Carlo method with discrete difference schemes. Numerical experiments involving some two-dimensional problems confirm the efficiency of the probabilistic scheme. © 1990 Academic Press, Inc

I. INTRODUCTION

Monte Carlo methods for the solution of elliptic partial differential equations have two advantages over standard deterministic techniques. First, they can efficiently be implemented on massively parallel computers. Second, it is possible to obtain the solution at a few points using a small fraction of the computer time needed to obtain the solution in the full domain. For many problems this second point is not important, however, there are problems where it is. For example, Thompson and Chen [1] employed probabilistic techniques to find economical approximations for local and "hot spot" temperatures in nuclear reactor components. Also, the probabilistic scheme can be very useful for solving problems that involve a severe gradient near a boundary point. In this case, finite difference schemes such as multigrid perform poorly; however, the Monte Carlo method can adequately approximate local behavior even in the presence of a steep gradient.

In this paper we consider a Monte Carlo method for solving Poisson's equation with Dirichlet boundary conditions:

$$\begin{aligned}\nabla^2 u(\mathbf{x}) &= -q(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) &= f(\mathbf{x}), & \mathbf{x} \in \partial\Omega\end{aligned}\tag{1}$$

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The principles for solving Eq. (1) via discrete random walks on a grid are well known; see, for example, Hammersley and Handscomb [2], Klahr [3], or Bauer [4]. Since the discrete random walk generally requires a large number of steps to reach the boundary (see Haji-Sheikh [5]), an alternative method, the random “walk on spheres” may be used to reduce the amount of computation. Brown [6] and Muller [7] employed this technique to solve Laplace’s equation. Also, Haji-Sheikh and Sparrow [8] applied this method to Poisson’s equation for a nonzero constant source term q . To obtain solutions to homogeneous elliptic partial differential equations with constant coefficients, Booth [9, 10] considered a scheme that involved a weighted, random “walk on spheres.” For problems involving a nonconstant source term, the difficulty lies in estimating internal contributions without tracing particle trajectories or resorting to numerical integration. A method for taking into account the right-hand side of Poisson’s equation has been developed by Mikhailov and Elepov [11]. The technique is based on a “one-point random estimation inside the sphere.” A description of these methods and bounds on the runtime of the algorithm is contained in the books by Elepov *et al.* [12] and Sabelfeld [13]. In this paper, we present a new method for analyzing the performance of this algorithm. The basic idea involves relating the average number of steps in the random walk to a specific Dirichlet problem for Poisson’s equation and then deriving an upper bound for the integral representation of the solution to this problem. We use the estimates of the runtime and the results of numerical experiments to compare the Monte Carlo method with discrete difference schemes.

For the sake of completeness, we review the modified “walk on spheres” algorithm for Poisson’s equation with nonconstant source term q . We begin by outlining the procedure for estimating the solution $u(\mathbf{x}_0)$ at an interior point \mathbf{x}_0 and then in the next section we discuss the algorithm more formally. Let us denote by $S(\mathbf{x}_0)$ the largest sphere centered at \mathbf{x}_0 and entirely contained in Ω . To approximate $u(\mathbf{x}_0)$ a point \mathbf{x}_1 is chosen uniformly on the sphere $S(\mathbf{x}_0)$ and a second point \mathbf{y}_1 inside $S(\mathbf{x}_0)$ is selected with respect to the density related to the Green’s function for the ball (See Fig. 1). The contribution from sources inside the ball is estimated by the weighted score $a(\mathbf{x}_0)q(\mathbf{y}_1)$, where $a(\mathbf{x}_0)$ is the normalizing constant with respect to the Green’s function. If \mathbf{x}_1 is close to the boundary, say within δ , then $u(\mathbf{x}_1)$ can be approximated by the evaluating $f(\mathbf{x})$ at a nearby boundary point. The estimate of $u(\mathbf{x}_0)$ produced by one particle is then $u(\mathbf{x}_1) + a(\mathbf{x}_0)q(\mathbf{y}_1)$. Usually \mathbf{x}_1 will not lie within δ of $\partial\Omega$, so that $u(\mathbf{x}_1)$ is not known. In this case we estimate $u(\mathbf{x}_1)$ in the same way as before; that is, we sample \mathbf{x}_2 uniformly from the largest sphere $S(\mathbf{x}_1)$ (centered at \mathbf{x}_1) contained in Ω and we select a point \mathbf{y}_2 inside $S(\mathbf{x}_1)$ according to the distribution induced by the Green’s function for the ball (See Fig. 1). Our approximation for $u(\mathbf{x}_1)$ is the sum $u(\mathbf{x}_2) + a(\mathbf{x}_1)q(\mathbf{y}_2)$. Replacing $u(\mathbf{x}_1)$ in the previous estimate leads to the approximation $u(\mathbf{x}_2) + a(\mathbf{x}_1)q(\mathbf{y}_2) + a(\mathbf{x}_0)q(\mathbf{y}_1)$. The procedure is repeated until the walk terminates at a point \mathbf{x}_n that lies within δ of $\partial\Omega$. The estimate of the solution at \mathbf{x}_0 given by one particle is then $u(\mathbf{x}_n) + a(\mathbf{x}_{n-1})q(\mathbf{y}_n) + \cdots + a(\mathbf{x}_0)q(\mathbf{y}_1)$. Averaging over several trials provides an increasingly more accurate approximation for the value $u(\mathbf{x}_0)$.

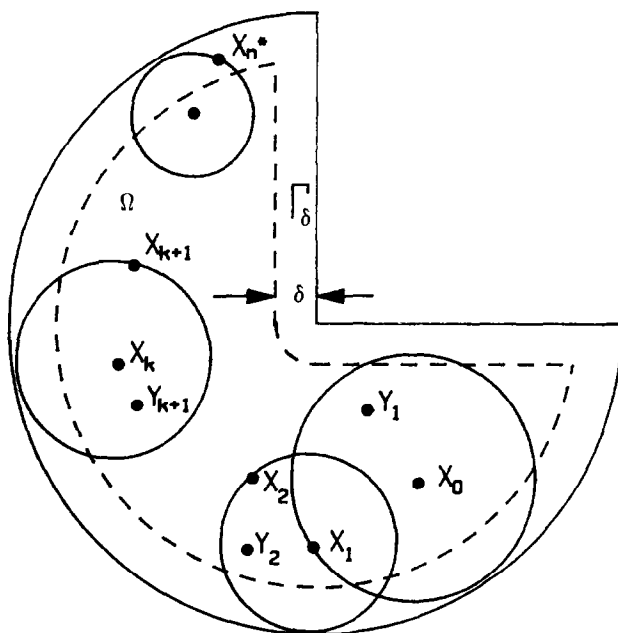


FIG. 1. Modified walk on spheres.

The operation count of the algorithm is partially determined by the number of steps required for the particle to reach the boundary. We will show that the average number of such steps is on the order of $|\ln \delta|$. Also, assuming that $u(\mathbf{x})$ can be adequately approximated by boundary values whenever \mathbf{x} is close to the boundary, we show that in order for the simulation to achieve a variance of size N^{-1} , an average of $O(N \ln N)$ number of operations are required. Here, N is the number of particles or trials.

It is instructive to compare the "walk on spheres" with the discrete random walk and finite difference schemes for a ν -dimensional grid of side length M^{-1} . The very best difference methods (such as a fast Poisson solver or multigrid) require at least $O(M^\nu)$ operations to achieve an accuracy of $O(M^{-2})$. It is known that the discrete random walk performs on average $O(M^2)$ steps before exiting the domain and that the standard deviation of the simulation for M^4 walks is $O(M^{-2})$, see, for example, Feynman [14, Vol. I, Section 41-4]. It follows that to produce a standard deviation of size $O(M^{-2})$ the discrete random walk requires on average $O(M^6)$ operations. On the other hand, to achieve a standard deviation on the order of M^{-2} , we will show that the walk on spheres requires only $O(M^4 \ln M)$ operations. Here, the number of particles or trials is $O(M^4)$ and δ is chosen to be $O(M^{-p})$ for some $p > 0$. This procedure clearly outperforms the discrete walk and compares favorably with difference schemes for $\nu \geq 4$. (Let us compare this procedure with the modified Monte Carlo scheme that numerically evaluates the integrals of the source q with

respect to the Green's function for the ball. It can be shown that, in this case, a simulation which uses $O(M^4)$ particles or walks has a standard deviation of approximately $O(M^{-2})$. Assuming only that q is continuous, most of the integrations would require at least $O(M^2)$ operations to produce an accuracy of $O(M^{-2})$. Although the integral associated with the first step need only be calculated once, most of the integrals associated with the remaining $O(|\ln \delta|) = O(\ln M)$ steps must be evaluated for each walk. It follows that a Monte Carlo method using this prescription would require roughly $O(M^6 \ln M)$ operations.) It is worth noting that the number of operations for the "walk on spheres" remains the same in higher dimensions whereas the operation count for finite difference methods increases at least linearly with the number of grid points. So the procedure becomes more attractive the higher the dimension. In addition, the algorithm can be implemented on a massively parallel machine in a straightforward manner.

The next section describes more precisely our modified walk on spheres. In the third section we derive an upper bound for the average number of steps required to reach the boundary. Also we present a bound on the variance of the process. The method of proof used here is new. The fourth section provides the results of some numerical experiments.

II. MODIFIED RANDOM WALK

For this discussion we assume that the boundary $\partial\Omega$ is sufficiently smooth so as to ensure the existence of a unique solution $u(\mathbf{x})$ that is twice continuously differentiable in Ω and continuous on $\Omega \cup \partial\Omega$. Also we assume that q is continuous in $\Omega \cup \partial\Omega$ and that the domain Ω consists of a finite union of bounded convex sets. In addition, we suppose that the Green's function $G_\Omega(\mathbf{x}, \mathbf{x}_0)$ for the Dirichlet problem on Ω exists and that it is continuously differentiable for $\mathbf{x} \in \Omega \cup \partial\Omega - \{\mathbf{x}_0\}$. (It may be possible to prove our results under less restrictive assumptions; however, these conditions are sufficient.) To simplify the discussion, we focus our attention on two- and three-dimensional problems. It is known that the solution to Eq. (1), $u(\mathbf{x}_0)$, has the integral representation (see, for example, Garabedian [15], Zachmanoglou and Thoe [16], or Vladimirov [17])

$$u(\mathbf{x}_0) = \int_{B(\mathbf{x}_0)} q(\mathbf{x}) G(\mathbf{x}, \mathbf{x}_0) d\mathbf{x} + \frac{1}{|S(\mathbf{x}_0)|} \int_{S(\mathbf{x}_0)} u(\mathbf{x}) d\sigma, \quad (2)$$

where $B(\mathbf{x})$ is the largest ball contained in Ω and centered at \mathbf{x}_0 , $S(\mathbf{x}_0) = \partial B(\mathbf{x}_0)$ is the boundary of $B(\mathbf{x}_0)$, $|S(\mathbf{x}_0)|$ denotes the surface area of $B(\mathbf{x}_0)$, and $G(\mathbf{x}, \mathbf{x}_0)$ is the Green's function for the ball.

Equation (2) admits a probabilistic interpretation. The value $u(\mathbf{x}_0)$ at the center of the sphere is the average of $q(\mathbf{x})$ with respect to the Green's function for the ball plus the uniform average of the boundary values on the surface of the ball. If the boundary values on the sphere were known, $u(\mathbf{x}_0)$ could be estimated by randomly

sampling $q(\mathbf{x})$ inside the ball (to estimate the first integral) and uniformly selecting $u(\mathbf{x})$ on the sphere (to estimate the second integral). Averaging over a large number of trials and summing would give an estimate of $u(\mathbf{x}_0)$. The method for solving a more general boundary value problem is an extension of this procedure.

To write the preceding considerations more formally, we introduce some notation. Let $d = d(\mathbf{x}_0)$ denote the minimum distance from \mathbf{x}_0 to the boundary $\partial\Omega$ ($d(\mathbf{x}_0)$ is the radius of $B(\mathbf{x}_0)$) and set $\rho(\mathbf{x}, \mathbf{x}_0)$ equal to the density (in rectangular coordinates) associated with the Green's function (for the Dirichlet problem) for the ball centered at \mathbf{x}_0 with radius d , namely,

$$\rho(\mathbf{x}, \mathbf{x}_0) = G(\mathbf{x}, \mathbf{x}_0)/a(\mathbf{x}_0), \quad (3)$$

where

$$a(\mathbf{x}_0) = \int_{B(\mathbf{x}_0)} G(\mathbf{x}, \mathbf{x}_0) d\mathbf{x};$$

here $a(\mathbf{x}_0) = d^2/4$, $d^2/6$ in two and three dimensions, (Zachmanoglou and Thoe [16], Sections 7.9 and 7.10), respectively. In two dimensions the density is given by (Zachmanoglou and Thoe [16])

$$\rho(r, \theta) = \frac{2r}{\pi d^2} \ln \frac{d}{r}, \quad 0 \leq r \leq d, \quad (4)$$

where (r, θ) , $0 \leq \theta \leq 2\pi$, is the polar coordinate representation of a point in a reference frame with the origin placed at \mathbf{x}_0 . Notice that $\rho(r, \theta)$ is circular symmetric, so that θ is selected uniformly from $0 \leq \theta \leq 2\pi$ and r is chosen according to the density given on the right-hand side of identity (4). The three-dimensional density is given by (Zachmanoglou and Thoe [16])

$$\rho(r, \theta, \phi) = \frac{3}{2\pi d^3} r(d-r) \sin \phi, \quad 0 \leq r \leq d, \quad (5)$$

where (r, θ, ϕ) , $0 \leq \theta \leq 2\pi$, $0 \leq \phi \leq \pi$, is the representation in spherical coordinates of a point in a system with the origin located at \mathbf{x}_0 .

Now, suppose X denotes a uniformly distributed random variable on the sphere $S(\mathbf{x})$ and Y designates a random variable with density $\rho(\mathbf{x}, \mathbf{x}_0)$. Using the definition of $\rho(\mathbf{x}, \mathbf{x}_0)$ and $a(\mathbf{x}_0)$, the integral representation (2) can be rewritten as

$$u(\mathbf{x}_0) = a(\mathbf{x}_0) Eq(Y) + Eu(X), \quad (6)$$

here E denotes expected value. The first term is a weighted average taken with respect to the Green's function and represents the expected contribution from sources inside the ball. The second term describes a mean value with respect to a

uniform distribution on the sphere and represents the average score upon exiting the ball $B(\mathbf{x}_0)$.

The uniform density and the density $\rho(\mathbf{x}, \mathbf{x}_0)$ can be used to construct transition probabilities for a markov chain. The transition from an initial point $X_0 = \mathbf{x}_0$ is performed by uniformly selecting a point X_1 on the sphere $S(\mathbf{x}_0)$ and by generating a random variable Y_1 with density $\rho(\mathbf{x}, \mathbf{x}_0)$. Given the position $X_k = \mathbf{x}_k$ at the k th step the transition to the $(k + 1)$ th step is carried out by choosing X_{k+1} uniform on the sphere $S(\mathbf{x}_k)$ and by selecting Y_{k+1} according to the density $\rho(\mathbf{y}, \mathbf{x}_k)$ (X_{k+1} and Y_{k+1} are independent of one another) see Fig. 1. The "walk on spheres" is simulated by repeating this procedure until the particle exits the domain. For the points X_k the solution $u(\mathbf{x})$ must satisfy Eq. (6); that is, with probability one

$$u(X_k) = a(X_k) E[q(Y_{k+1}) | X_k] + E[u(X_{k+1}) | X_k]; \quad (7)$$

here conditional expectations are used because the densities are determined by the position of X_k .

Roughly, the connection between the solution to the Dirichlet problem and the random process follows from the telescoping sum

$$\begin{aligned} u(\mathbf{x}_0) &= Eu(X_0) = Eu(X_n) + \sum_{k=0}^{n-1} E[u(X_k) - u(X_{k+1})] \\ &= Eu(X_n) + \sum_{k=0}^{n-1} E\{u(X_k) - E[u(X_{k+1}) | X_k]\}, \end{aligned} \quad (8)$$

where $X_0 = \mathbf{x}_0$. In the last equality we have used the fact that $E\{E[u(X_{k+1}) | X_k]\} = E[u(X_{k+1})]$, see, for example, Breiman [17, p. 75]. Applying identity (7) yields

$$u(\mathbf{x}_0) = Eu(X_n) + \sum_{k=0}^{n-1} E[a(X_k) q(Y_{k+1})]. \quad (9)$$

Now, suppose the process hits the boundary on the n th step, then all the terms on the right-hand side of equation (9) would be known. This suggests that $u(\mathbf{x}_0)$ is the mean value of the exit points plus a weighted average from internal contributions.

The Monte Carlo method makes use of the preceding observation to estimate $u(\mathbf{x}_0)$. However, the probabilistic scheme as stated cannot be realized numerically because the process almost surely (with probability one) does not reach the boundary in a finite number of steps. To limit the number of steps we end the walk whenever it gets to within some distance $d(\mathbf{x}) \leq \delta$ of the boundary and we assume that the solution can be well approximated by a nearby point on the boundary (the error can be estimated as per Booth [10]). In other words, we assume that the solution to the Dirichlet problem on the set (see Fig. 1)

$$\Gamma_\delta = \{\mathbf{x} \in \Omega \cup \partial\Omega: d(\mathbf{x}) < \delta\} \quad (10)$$

can be adequately approximated by values $f(\mathbf{x}')$ along the boundary (here \mathbf{x}' is chosen so that $|\mathbf{x}' - \mathbf{x}| = d(\mathbf{x})$), and we terminate the process whenever $X_n \in \Gamma_\delta$. Also, we define

$$n^* = \min\{n: X_n \in \Gamma_\delta\}, \quad (11)$$

as the stopping time for the random walk. To see that $P(n^* < +\infty) = 1$ we notice that at each step there is a positive (possibly small) probability that the process will terminate. This probability is bounded below by some positive constant, say $P(\delta)$. The probability that the process terminates is greater than or equal to the probability of at least one success in an infinite sequence of Bernoulli trials with probability of success at each trial given by $P(\delta)$. Since the latter occurs with probability one, it follows that $P(n^* < +\infty) = 1$.

To demonstrate the relationship between $u(\mathbf{x}_0)$ and the process that terminates whenever the particle's distance to the boundary is less than δ we proceed as before (except that n is replaced by n^*), set $X_0 = \mathbf{x}$ and write $u(\mathbf{x}_0)$ as a collapsing sum to obtain

$$\begin{aligned} u(\mathbf{x}_0) &= Eu(X_0) \\ &= Eu(X_{n^*}) + E\left(\sum_{k=0}^{n^*-1} [u(X_k) - u(X_{k+1})]\right) \\ &= Eu(X_{n^*}) + E\left(\sum_{k=0}^{n^*-1} \{u(X_k) - E[u(X_{k+1})|X_k]\}\right). \end{aligned} \quad (12)$$

The last step follows by using standard arguments for conditional expectations, Breiman [18]. Next, applying identity (7) yields

$$u(\mathbf{x}_0) = Eu(X_{n^*}) + E\left[\sum_{k=0}^{n^*-1} a(X_k) q(Y_{k+1})\right]. \quad (13)$$

(The main difference between Eqs. (9) and (13) is the random upper limit $n^* - 1$. To prove results about the algorithm, it is not sufficient to derive expressions for a fixed epoch n as in equation (9), we must also analyze expressions involving the random stopping time n^* . The presence of the random variable n^* in Eqs. (12) and (13) requires that we use a slightly different argument than the one given in Eqs. (8) and (9); see Breiman [18].) Using the approximation $Eu(X_{n^*}) \approx Ef(X_{n^*})$, with f evaluated at a point close to X_{n^*} , leads to

$$u(\mathbf{x}_0) \approx Ef(X_{n^*}) + E\left[\sum_{k=0}^{n^*-1} a(X_k) q(Y_{k+1})\right]. \quad (14)$$

In other words, we have shown that the solution to the boundary value problem at \mathbf{x}_0 approximately equals the expected contribution from the "exit points" plus the mean value of a weighted average for the internal contributions $q(Y_{k+1})$.

At the conclusion of each walk we compute the random sample

$$Z_i = f(X_{n^*}^i) + \sum_{k=0}^{n^*-1} a(X_k^i) q(Y_{k+1}^i), \quad (15)$$

where i denotes the i th experiment. By Eqs. (14) and (15) we have $EZ_i \approx u(\mathbf{x}_0)$. An estimate for the mean of Z_i is given by the statistic

$$S_N = \frac{1}{N} \sum_{i=1}^N Z_i, \quad (16)$$

where N is the number of trials. By the law of large numbers S_N approximates $u(\mathbf{x}_0)$ for N sufficiently large.

The duration of the random walk and the rate at which S_N converges determine the computing time for the algorithm. Here and in the following we will assume that \mathbf{x}_0 is fixed and that δ is considerably smaller than $d(\mathbf{x}_0)$. Assuming that the domain consists of a finite union of bounded convex regions we demonstrate

LEMMA. *For random walks originating at $\mathbf{x}_0 \in \Omega - \Gamma_\delta$,*

$$En^* = O(|\ln \delta|) \text{ and } \text{Var } Z_i = O(1), \text{ as } \delta \rightarrow 0, \quad (17)$$

$$\text{with } n^* = \min\{n: d(X_n) < \delta\} \text{ and } Z_i = f(X_{n^*}^i) + \sum_{k=0}^{n^*-1} a(X_k^i) q(Y_{k+1}^i).$$

The proof of the lemma is deferred to the next section.

The preceding result implies that on average the walks are of short duration. For example, suppose $\delta = N^{-p}$ with $p > 0$, the expected length of the walk is only on the order of $\ln N$.

The bound on $\text{Var } Z_i$ provides an estimate for the rate at which S_N converges; that is,

$$\text{Var } S_N = N^{-2} \sum_{i=1}^N \text{Var } Z_i = O(N^{-1}). \quad (18)$$

Here we have used the independence of the Z_i 's, i.e., $\text{Cov}(Z_i, Z_j) = 0$, $i \neq j$. Expression (18) shows that S_N converges in mean square to EZ_i at the rate $O(N^{-1})$.

Recall from Eqs. (14) and (15) that $EZ_i \approx u(\mathbf{x}_0)$ and that the error in this approximation was introduced by the estimate $Eu(X_{n^*}) \approx Ef(X_{n^*})$. To quantify this error we make the assumption that $|Eu(X_{n^*}) - Ef(X_{n^*})| = O(\delta^{1/p})$ as $\delta \rightarrow 0$ for some $p > 0$. This assumption holds true (although not demonstrated here), for example,

whenever u is continuously differentiable over $\Omega \cup \partial\Omega$. Under this assumption we can use Eqs. (13), (15), (16), and (18) to derive

$$\begin{aligned} E[S_N - u(\mathbf{x}_0)]^2 &= E \left\{ S_N - ES_N + \frac{1}{N} \sum_{i=1}^N [Ef((X_{n^*}^i) - Eu(X_{n^*}^i))] \right\}^2 \\ &\leq 2E(S_N - ES_N)^2 + \frac{2}{N^2} \left\{ \sum_{i=1}^N |Ef(X_{n^*}^i) - Eu(X_{n^*}^i)| \right\}^2 \\ &\leq 2 \text{Var } S_N + 2[Ef(X_{n^*}^1) - Eu(X_{n^*}^1)]^2 = O(N^{-1} + \delta^{2/p}), \end{aligned} \tag{19}$$

here we have used the inequality $(A + B)^2 \leq 2A^2 + 2B^2$ and the fact that the random variables $X_{n^*}^i$ have the same distribution. In other words, we have shown that the statistic S_N converges in mean square to $u(\mathbf{x}_0)$ at the rate $O(N^{-1} + \delta^{2/p})$. Assuming the validity of the lemma we have

THEOREM. For $\delta = N^{-p/2}$ the statistic S_N converges in mean square to the solution $u(\mathbf{x}_0)$ at the rate $O(N^{-1})$ and the average operation count for the simulation is $O(N \ln N)$.

The average operation count is derived by multiplying the number of experiments by the expected number of steps in a random walk.

III. BOUNDS ON EXPECTED STOPPING TIME AND VARIANCE

The proof of the lemma is based on a specific Dirichlet problem for Poisson's equation. Notice that the length of the walk, n^* , depends only on the domain; that is, the duration of the walk does not depend on the solution to a particular problem given by Eq. (1). So we may consider the problem given by

$$\begin{aligned} \nabla^2 w(\mathbf{x}) &= -q(\mathbf{x}), & \mathbf{x} \in \Omega \\ w(\mathbf{x}) &= 0, & \mathbf{x} \in \partial\Omega, \end{aligned} \tag{20}$$

where $q(\mathbf{x}) = d(\mathbf{x})^{-2}$, $\mathbf{x} \in \Omega - \Gamma_\delta$, $q(\mathbf{x}) = \delta^{-2}$, $\mathbf{x} \in \Gamma_\delta$, and Ω is the same as in Eq. (1). It is known that (see, for example, Vladimirov [17])

$$w(\mathbf{x}_0) = \int_{\Omega} q(\mathbf{x}) G_{\Omega}(\mathbf{x}, \mathbf{x}_0) d\mathbf{x}. \tag{21}$$

In the above, $G_{\Omega}(\mathbf{x}, \mathbf{x}_0)$ is the Green's function for the Dirichlet problem on $\Omega \cup \partial\Omega$. The bound on En^* is derived by estimating $w(\mathbf{x}_0)$.

To see this, we first notice that $w(\mathbf{x}_0) \geq 0$, since $G_{\Omega}(\mathbf{x}, \mathbf{x}_0) \geq 0$ for $(\mathbf{x} \neq \mathbf{x}_0)$

(Zachmanoglou and Thoe [16]) and $q(\mathbf{x}) \geq 0$ in Eq. (21). Next we observe from expression (13),

$$\begin{aligned}
 w(\mathbf{x}_0) &= Ew(X_{n^*}) + E \left[\sum_{k=0}^{n^*-1} a(X_k) q(Y_{k+1}) \right] \\
 &\geq E \left[\sum_{k=0}^{n^*-1} a(X_k) q(Y_{k+1}) \right].
 \end{aligned}
 \tag{22}$$

Recalling the inequality $a(\mathbf{x}) \geq d(\mathbf{x})^2/6$ from Eq. (3) (for two- and three-dimensional problems), the definition of $q(\mathbf{x}) = \min\{\delta^{-2}, d(\mathbf{x})^{-2}\}$ in Eq. (20) and the fact that $d(Y_{k+1}) \leq 2d(X_k)$ (see Fig. 1) leads to the lower bound $a(X_k) q(Y_{k+1}) \geq c$, for some positive constant c . It follows from expression (22)

$$w(\mathbf{x}_0) \geq cEn^*,
 \tag{23}$$

which is the desired inequality. In the following c and c' will denote (not necessarily the same constants each time they appear) positive constants.

The maximum of the upper bounds for the integral in identity (21) over each convex subregion provides a bound on $w(\mathbf{x}_0)$. The asymptotic analysis for the convex region containing \mathbf{x}_0 is analogous to the argument for the other convex subregions, so we may assume that Ω is convex. Let us partition Ω into three subsets

$$\begin{aligned}
 w(\mathbf{x}_0) &= \int_B + \int_{\Omega - \Gamma_\delta - B} + \int_{\Gamma_\delta} q(\mathbf{x}) G_\Omega(\mathbf{x}, \mathbf{x}_0) d\mathbf{x}, \\
 &= I_1 + I_2 + I_3,
 \end{aligned}
 \tag{24}$$

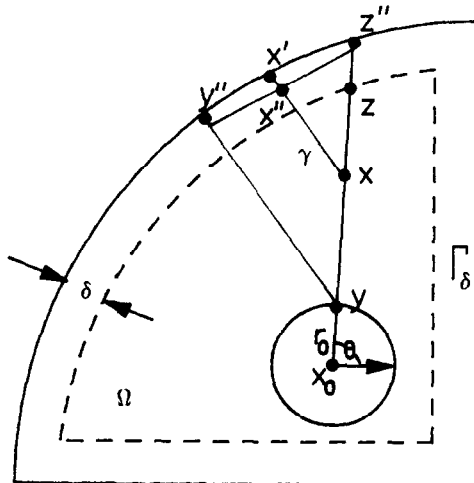


FIG. 2. Diagram for estimation of integrals.

here B is a ball centered at \mathbf{x}_0 with radius $r_0 = d(\mathbf{x}_0)/2$, see Fig. 2. We establish bounds for each of these integrals in the two-dimensional case, the three-dimensional case is similar.

We begin by recalling the definition of the Green's function $G_\Omega(\mathbf{x}, \mathbf{x}_0)$ for the Dirichlet problem on $\Omega \cup \partial\Omega$ (Zachmanoglou and Thoe [16, Sect. 7.9])

$$\begin{aligned} G_\Omega(\mathbf{x}, \mathbf{x}_0) &= \frac{1}{2\pi} \ln |\mathbf{x} - \mathbf{x}_0| + g(\mathbf{x}, \mathbf{x}_0), & \mathbf{x} \in \Omega \\ G_\Omega(\mathbf{x}, \mathbf{x}_0) &= 0, & \mathbf{x} \in \partial\Omega \end{aligned} \tag{25}$$

here $g(\mathbf{x}, \mathbf{x}_0)$ is harmonic in Ω and $g(\mathbf{x}, \mathbf{x}_0) = -\frac{1}{2}\pi \ln |\mathbf{x} - \mathbf{x}_0|$ for $\mathbf{x} \in \partial\Omega$. We have assumed that $g(\mathbf{x}, \mathbf{x}_0)$ is continuously differentiable on $\Omega \cup \partial\Omega$.

(1) For the integral I_1 over the region B , we observe that the functions $q(\mathbf{x})$ and $g(\mathbf{x}, \mathbf{x}_0)$ are bounded so we need only estimate $\int_B \ln |\mathbf{x} - \mathbf{x}_0| d\mathbf{x}$. The latter can be evaluated and is finite.

Before proceeding with the analysis of the integrals I_2 and I_3 over the regions $\Omega - \Gamma_\delta - B$ and Γ_δ , respectively, we estimate the rate at which $G_\Omega(\mathbf{x}, \mathbf{x}_0)$ goes to zero as \mathbf{x} approaches the boundary. For $\mathbf{x} \in \Omega - B$ we will show that

$$G_\Omega(\mathbf{x}, \mathbf{x}_0) \leq c d(\mathbf{x}). \tag{26}$$

Since, by assumption, $g(\mathbf{x}, \mathbf{x}_0)$ has bounded first derivative, a first order expansion of the function $v(s) = g(\mathbf{x} + (1-s)(\mathbf{x}' - \mathbf{x}), \mathbf{x}_0)$ in the variable s leads to

$$\begin{aligned} g(\mathbf{x}, \mathbf{x}_0) &= v(1) = v(0) + O(|\mathbf{x}' - \mathbf{x}|), \\ &= g(\mathbf{x}', \mathbf{x}_0) + O(|\mathbf{x}' - \mathbf{x}|), \\ &= -\frac{1}{2\pi} \ln |\mathbf{x}' - \mathbf{x}_0| + O[d(\mathbf{x})], \end{aligned} \tag{27}$$

where \mathbf{x}' is a point on the boundary $\partial\Omega$ chosen so that $d(\mathbf{x}) = |\mathbf{x}' - \mathbf{x}|$, see Fig. 2. Substituting this expression into Eq. (25) produces

$$G_\Omega(\mathbf{x}, \mathbf{x}_0) = \frac{1}{2\pi} \ln \frac{|\mathbf{x} - \mathbf{x}_0|}{|\mathbf{x}' - \mathbf{x}_0|} + O[d(\mathbf{x})]. \tag{28}$$

Using the inequality $|\mathbf{x} - \mathbf{x}_0| \leq |\mathbf{x} - \mathbf{x}'| + |\mathbf{x}' - \mathbf{x}_0|$ and the estimate $\ln(1 + \eta) = O(\eta)$, $\eta > 0$, we obtain the bound

$$\begin{aligned} \ln \frac{|\mathbf{x} - \mathbf{x}_0|}{|\mathbf{x}' - \mathbf{x}_0|} &\leq \ln \left(1 + \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x}' - \mathbf{x}_0|} \right) \\ &= O \left(\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x}' - \mathbf{x}_0|} \right) = O[d(\mathbf{x})]. \end{aligned} \tag{29}$$

Replacing the first term in Eq. (28) by expression (29) we arrive at inequality (26).

(2) To bound the integral I_2 we use the definition of $q(\mathbf{x}) = d(\mathbf{x})^{-2}$ on $\Omega - \Gamma_\delta$ and expression (26) to derive

$$\begin{aligned} I_2 &= \int_{\Omega - \Gamma_\delta - B} q(\mathbf{x}) G_\Omega(\mathbf{x}, \mathbf{x}_0) d\mathbf{x} \\ &\leq c \int_{\Omega - \Gamma_\delta - B} d(\mathbf{x})^{-1} d\mathbf{x}. \end{aligned} \quad (30)$$

Next, we change the independent variables from rectangular coordinates to polar coordinates (r, θ) with \mathbf{x}_0 treated as the origin. Let us consider a ray that originates at \mathbf{x}_0 and has angle θ . We set \mathbf{y} and \mathbf{z} equal to the points of intersection of the ray with ∂B and $\partial\Gamma_\delta \cap \Omega$, respectively (see Fig. 2) and define $R(\theta) = |\mathbf{z} - \mathbf{x}_0|$ (notice that $|\mathbf{y} - \mathbf{x}_0| = r_0$). Also, we observe that $R(\theta)$ is bounded by some constant, say the maximal chord length or diameter D . The integral on the right-hand side of expression (30) can be rewritten as

$$\begin{aligned} \int_{\Omega - \Gamma_\delta - B} d(\mathbf{x})^{-1} d\mathbf{x} &= \int_0^{2\pi} \int_{r_0}^{R(\theta)} d(\mathbf{x})^{-1} r dr d\theta, \\ &\leq D \int_0^{2\pi} \int_{r_0}^{R(\theta)} d(\mathbf{x})^{-1} dr d\theta \end{aligned} \quad (31)$$

here \mathbf{x} is the point corresponding to (r, θ) .

To proceed we will need the following bound for $d(\mathbf{x})^{-1}$,

$$d(\mathbf{x})^{-1} \leq \frac{D}{r_0} |\mathbf{z}'' - \mathbf{x}|^{-1}, \quad (32)$$

where \mathbf{z}'' is the intersection of the ray through \mathbf{z} (originating at \mathbf{x}_0) with $\partial\Omega$, see Fig. 2. To this end we set \mathbf{x}' equal to a point satisfying $d(\mathbf{x}) = |\mathbf{x}' - \mathbf{x}|$ and construct the line segment γ between \mathbf{x} and \mathbf{x}' , see Fig. 2. Let us consider the half-plane containing \mathbf{x}' and the line through \mathbf{y} and \mathbf{z} (the line forms the boundary of the half-plane). We introduce the half-line (contained in the half-plane) that starts at \mathbf{y} and is parallel to γ . Let us denote by \mathbf{y}'' the intersection of the half-line with $\partial\Omega$, see Fig. 2 (notice that $|\mathbf{y} - \mathbf{y}''|$ is bounded away from zero, in fact, $|\mathbf{y} - \mathbf{y}''| \geq d(\mathbf{x}_0)/2 = r_0$). Since $\Omega \cup \partial\Omega$ is convex, the chord between \mathbf{y}'' and \mathbf{z}'' must lie in $\Omega \cup \partial\Omega$ and, therefore, it intersects the line segment γ , say at the point \mathbf{x}'' , see Fig. 2. Because the triangles with vertices $\{\mathbf{y}, \mathbf{y}'', \mathbf{z}''\}$ and $\{\mathbf{x}, \mathbf{x}'', \mathbf{z}''\}$ are similar,

$$\frac{|\mathbf{z}'' - \mathbf{x}|}{|\mathbf{x}'' - \mathbf{x}|} = \frac{|\mathbf{z}'' - \mathbf{y}|}{|\mathbf{y}'' - \mathbf{y}|} \leq \frac{D}{r_0} \quad (33)$$

and, since $|\mathbf{x}'' - \mathbf{x}| \leq |\mathbf{x}' - \mathbf{x}| = d(\mathbf{x})$, it follows that

$$d(\mathbf{x})^{-1} \leq |\mathbf{x}'' - \mathbf{x}|^{-1} \leq \frac{D}{r_0} |\mathbf{z}'' - \mathbf{x}|^{-1} \tag{34}$$

as desired.

Applying inequality (32) to the inside integral on the right-hand side of inequality (31), we obtain

$$\int_{r_0}^{R(\theta)} d(\mathbf{x})^{-1} dr \leq \frac{D}{r_0} \int_{r_0}^{R(\theta)} |\mathbf{z}'' - \mathbf{x}|^{-1} dr; \tag{35}$$

here \mathbf{z}'' is a function of θ and \mathbf{x} corresponds to (r, θ) . Now, a change in the variable of integration to $t = R(\theta) - r + \delta$ or $r = R(\theta) - t + \delta$ produces

$$\begin{aligned} \int_{r_0}^{R(\theta)} |\mathbf{z}'' - \mathbf{x}|^{-1} dr &= \int_{\delta}^{R(\theta) - r_0 + \delta} |\mathbf{z}'' - \mathbf{x}|^{-1} dt \\ &\leq \int_{\delta}^{R(\theta) - r_0 + \delta} t^{-1} dt. \end{aligned} \tag{36}$$

The inequality follows from the observations:

$$|\mathbf{z}'' - \mathbf{x}| = |\mathbf{z}'' - \mathbf{z}| + |\mathbf{z} - \mathbf{x}| \geq \delta + [R(\theta) - r] = t. \tag{37}$$

The last integral in expression (36) is $O(|\ln \delta|)$, as desired.

(3) To provide a bound for the integral I_3 over Γ_δ we notice that the area of Γ_δ is bounded by δL , where L is the arc length of $\partial\Omega$ (see, for example, Courant and John [19, section 4.10]). Using expression (26) and the fact that $d(\mathbf{x}) \leq \delta$ for $\mathbf{x} \in \Gamma_\delta$ produces the inequality

$$\int_{\Gamma_\delta} q(\mathbf{x}) G_\Omega(\mathbf{x}, \mathbf{x}_0) d\mathbf{x} \leq c \int_{\Gamma_\delta} \delta^{-2} d(\mathbf{x}) d\mathbf{x} \leq c \delta^{-1} \int_{\Gamma_\delta} d\mathbf{x} \leq cL.$$

This completes the proof of the first part of the lemma, namely $En^* = O(|\ln \delta|)$.

To finish the proof of the lemma we must analyze the variance of $Z_i = f(X_{n^*}^i) + \sum_{k=0}^{n^*-1} a(X_k^i) q(Y_{k+1}^i)$, where f and q are from the original problem given by Eq. (1). Because f is bounded, the problem can be reduced to finding the bound for $E[\sum_{k=0}^{n^*-1} a(X_k) q(Y_{k+1})]^2$ (the Z_i 's have the same distribution so we can omit the superscript i). Since q is presumed bounded in Eq. (1) we need only estimate $E_1 = E[\sum_{k=0}^{n^*-1} a(X_k)]^2$. To this end we consider the specific Dirichlet problem given by Eq. (16) with $q = 1$. Using methods analogous to those given by expression (18) with $q = 1$, we obtain for a walk originating at \mathbf{x}

$$E_2 = E \left[\sum_{k=0}^{n^*-1} a(X_k) \mid X_0 = \mathbf{x} \right] \leq cw(\mathbf{x}). \tag{38}$$

In this case q is constant ($q = 1$) so that, by Eq. (21), $w(\mathbf{x})$ does not depend on δ . By virtue of the continuity of $w(\mathbf{x})$ (see Eq. (21)) the right-hand side of inequality (38) is bounded by some constant say c' for all $\mathbf{x} \in \Omega - \Gamma_\delta$. Because the inequality $E_2 \leq c'$ holds for an arbitrary starting point $\mathbf{x} \in \Omega - \Gamma_\delta$, we can replace the initial position by a random variable, say X_0 ,

$$E \left[\sum_{k=0}^{n^*-1} a(X_k) \mid X_0 \right] \leq c' \quad (39)$$

with probability one. Also, since $a(\mathbf{x}) \leq d(\mathbf{x}) \leq D$, it follows that

$$E \left[\sum_{k=0}^{n^*-1} a(X_k)^2 \mid X_0 = \mathbf{x}_0 \right] \leq DE_2 \leq Dc' = O(1). \quad (40)$$

Rewriting the term E_1 we arrive at the desired conclusion,

$$\begin{aligned} E \left[\sum_{k=0}^{n^*-1} a(X_k) \right]^2 &= 2E \left[\sum_{k=0}^{n^*-1} a(X_k) \sum_{j=k+1}^{n^*-1} a(X_j) \right] + E \left[\sum_{k=0}^{n^*-1} a^2(X_k) \right] \\ &= 2E \left\{ \sum_{k=0}^{n^*-1} a(X_k) E \left[\sum_{j=k+1}^{n^*-1} a(X_j) \mid X_k \right] \right\} + O(1) = O(1). \end{aligned} \quad (41)$$

Here, again, we have used the result for conditional expectations from Breiman [17]. The term $E[\sum_{j=k+1}^{n^*-1} a(X_j) \mid X_k]$ is bounded by the constant given in expression (39) with X_k as the initial position.

The key step in this argument is the introduction of the appropriate Dirichlet problem for Poisson's equation. In turn, the asymptotic analysis is reduced to estimating the solution to the boundary value problem. The desired approximations are then obtained from an integral representation of the solution.

IV. NUMERICAL EXPERIMENTS

Another indication of the performance of the algorithm was obtained through numerical experimentation. The problem chosen for this purpose involves a severe temperature gradient near the origin. In this case, a finite difference scheme like multigrid performs poorly whereas the Monte Carlo method is relatively unaffected. To demonstrate the usefulness of the probabilistic technique we also present a method for estimating the severity of the gradient.

The domain selected for this problem is the unit disk minus the first quadrant; that is, the set $\Omega = \{(r, \theta): 0 < r < 1, -3\pi/2 < \theta < 0\}$, see, for example, Fig. 1. We consider the poisson equation

$$\nabla^2 u = -(2 - r^2)e^{-r^2/2} \quad (42)$$

TABLE I

r	Theta	Actual solution	Monte Carlo	Error	Average no. steps
0.1244	-0.7906	0.8623	0.8672	0.0049	14.42
0.2320	-0.0274	0.9678	0.9626	0.0052	10.31
0.2187	-3.3975	0.4308	0.4377	0.0069	15.03
0.1476	-4.1617	0.4695	0.4806	0.0111	12.90
0.0129	-1.4790	0.8890	0.8854	0.0036	13.94

with a radially symmetric source $q(r, \theta) = (2 - r^2) \exp(-r^2/2)$. To obtain a comparison between numerical results and the actual solution, the function

$$u(r, \theta) = r^\alpha \sin(\alpha\theta) + e^{-r^2/2} \quad (43)$$

is taken as the solution to the Dirichlet problem, here $\alpha = \frac{1}{3}, \frac{2}{3},$ and 1. The boundary conditions are specified by the value of u on $\partial\Omega$. For $\alpha = \frac{1}{3}$ and $\frac{2}{3}$ the first term in expression (43) is not differentiable at the boundary. These values were chosen so as to reflect a temperature distribution u with a severe gradient at the origin.

First we let $\alpha = \frac{1}{3}$. In this case the boundary conditions are given by: $u(r, 0) = \exp(-r^2/2)$, $u(r, -3\pi/2) = -r^{1/3} + \exp(-r^2/2)$, and $u(1, \theta) = \sin(\theta/3) + e^{-1/2}$. The density $\rho(\mathbf{r}, \theta)$ used in the simulation is given by identity (4). Five points were selected uniformly from the intersection of Ω with the disk of radius $\frac{1}{4}$ centered at the origin. The walks were terminated when the distance to the boundary was less than $\delta = 5 \times 10^{-5}$ and $N = 500$ random walks were initiated from each point. For $\alpha = \frac{1}{3}$ the largest error introduced by the approximation $u(X_{n^*}) \approx f(X_{n^*})$ occurs near the origin. For this choice of δ the error is approximately $\delta^{1/3} \approx 0.04$. The statistic S_{500} was computed and the result was compared with the solution $u(r, \theta)$. In addition, the average number of steps for the "walk on spheres" was calculated for each point. The results are shown in Table I. (The initial points are given in polar coordinates (r, θ) .) After 500 trials all but one of the values produced by the simulation are within 10^{-2} of the actual solution. The experimental results are better than might be expected for this choice of δ ; however, a large number of walks terminate near the circular arc $r = 1$ and the error introduced there is very small, $\approx \delta$. So the average error produced by the approximation $u(X_{n^*}) \approx f(X_{n^*})$ is small.

Next we set $\alpha = \frac{2}{3}$. The boundary values are: $u(r, 0) = \exp(-r^2/2)$, $u(r, -3\pi/2) = \exp(-r^2/2)$, and $u(1, \theta) = \sin(2\theta/3) + e^{-1/2}$. In this case the term $r^{2/3} \sin(2\theta/3)$ vanishes along the rays $\theta = 0$ and $\theta = -3\pi/2$. This example is of interest because, even though $u(r, \theta)$ is well behaved for $\theta = 0, -3\pi/2$ (in fact it is analytic along these line segments) its derivative at the origin does not exist. A second experiment with $\alpha = \frac{2}{3}$, $N = 500$, and $\delta = 5 \times 10^{-5}$ was performed with the results shown in Table II. (In this case the error introduced near the origin is small since $\delta^{2/3} \approx 0.001$.) The initial points are the same as in the previous case. Most of the values lie within 10^{-2} of the correct solution.

TABLE II

r	Theta	Actual solution	Monte Carlo	Error	Average no. steps
0.1244	-0.7906	0.8670	0.8748	0.0078	14.42
0.2320	-0.0274	0.9665	0.9599	0.0066	10.31
0.2187	-3.3975	0.6973	0.7160	0.0187	15.03
0.1476	-4.1617	0.8889	0.9254	0.0365	12.90
0.0129	-1.4790	0.9541	0.9533	0.0008	13.94

Finally, we let $\alpha = 1$. This example was chosen to provide a comparison with a problem that has an analytical solution on the closure of the domain. As before we set $N = 500$ and $\delta = 5 \times 10^{-5}$. For $\alpha = 1$ the error produced by the approximation $u(X_{n^*}) \approx f(X_{n^*})$ is very small along the entire boundary $\approx \delta$. The results are given by Table III. Most of the values are within 10^{-2} of the analytical solution.

As an example of the usefulness of the probabilistic approach we present a procedure for estimating the "magnitude" of the gradient at the origin. Suppose that the solution to the Dirichlet problem for the domain given in the preceding examples is known to be of the form

$$u(r, \theta) = Ar^{2/3} \sin(2\theta/3) + F(r, \theta), \quad (44)$$

where F is twice continuously differentiable on $\Omega \cup \partial\Omega$ and A is not known. We refer to the unknown coefficient A as the "magnitude" of the gradient at the origin. To estimate A we use a first-order Taylor expansion in r for F and then, after solving for A , we obtain

$$A = \left[u(r, \theta) - F(0, \theta) - \frac{\partial}{\partial r} F(r, \theta) \Big|_{r=0} r \right] r^{-2/3} / \sin(2\theta/3) + O[r^{4/3} / \sin(2\theta/3)]. \quad (45)$$

The derivative $\partial F / \partial r$ is calculated from the known values along the rays $\theta = 0$ and $\theta = -3\pi/2$. An approximation for $u(r, \theta)$ is provided by the simulation. For

TABLE III

r	Theta	Actual solution	Monte Carlo	Error	Average no. steps
0.1244	-0.7906	0.9039	0.9096	0.0057	14.42
0.2320	-0.0274	0.9671	0.9592	0.0079	10.31
0.2187	-3.3975	0.0317	0.0518	0.0201	15.03
0.1476	-4.1617	0.1150	0.1427	0.0277	12.90
0.0129	-1.4790	0.9871	0.9919	0.0048	13.94

example, consider the solution at the point $(r, \theta) = (0.0129, -1.479)$ given in Table II (here $F(r, \theta) = \exp[-r^2/2]$). In this case

$$A \approx [0.9533 - 1.0]r^{-2.3}/\sin(2\theta/3) \approx 1.02, \quad (46)$$

whereas the constant A in Eq. (43) is one. So the procedure provides a good approximation for the magnitude of the gradient at zero.

V. SUMMARY

An efficient probabilistic scheme for approximating local solutions to Poisson's equation with a nonconstant source term has been developed by exploiting a modified random walk on spheres. A rigorous derivation for the rate of convergence and runtime of the simulation demonstrated that to achieve a variance of order N^{-1} requires on average $O(N \log N)$ operations. The technique represents a significant improvement in efficiency over other Monte Carlo methods for solving inhomogeneous source problems. Also, for estimating local solutions, the algorithm compares favorably with discrete difference schemes for ν -dimensional problems, $\nu \geq 4$. Another confirmation of the efficiency of the method was obtained by conducting some numerical experiments on a problem involving a severe temperature gradient near a boundary point. These experiments also indicate the method's ability to estimate the severity of the gradient.

In addition, the technique can be applied to other elliptic operators by introducing the appropriate Green's function. Problems involving certain other types of boundary conditions can be solved, for instance, by using methods developed for the simple random walk. The analysis of these and other methods is a subject of continuing research.

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