

# Monte Carlo Methods for Solving Elliptic Equations with Boundary Conditions Containing the Normal Derivative

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## 1. STATEMENT OF THE PROBLEM

Consider the following boundary value problem. Suppose that a function  $u_i(x)$  satisfies the Poisson equation

$$\epsilon_i \Delta u_i = -\rho \quad (1)$$

inside a bounded simply connected domain  $G_i \subset \mathbb{R}^3$  with simply connected boundary  $\Gamma$  and a function  $u_e(x)$  satisfies the homogeneous Poisson–Boltzmann linear equation

$$\epsilon_e \Delta u_e - \epsilon_e \kappa^2 u_e = 0 \quad (2)$$

on the exterior domain  $G_e = \mathbb{R}^3 \setminus \bar{G}_i$ ; the coefficient  $\kappa$  may be equal to zero, and  $\epsilon_e \geq \epsilon_i$ . On the boundary, compatibility conditions are imposed; namely, both the solution and the flow must be continuous when passing through the boundary:

$$u_i(g) = u_e(y), \quad \epsilon_i \frac{\partial u_i}{\partial n}(y) = \epsilon_e \frac{\partial u_e}{\partial n}(y), \quad y \in \Gamma. \quad (3)$$

We assume that the normal vector  $n$  is directed inside  $G_e$ .

The problem is to find the solution and its first derivatives at finitely many given points and evaluate energy, which can be represented in the form of a linear functional of the solution in the case under consideration. Similar problems arise in physical chemistry, when the electrostatic properties of individual molecules in an electrolyte solution are to be calculated.

The standard approach to constructing Monte Carlo estimators for solutions to boundary value problems for elliptic equations consists in applying the algorithm of

random walk on spheres [1, 2]. If the boundary condition contains the normal derivative, then a randomized finite-difference approximation to this derivative is used [3–6]. As a consequence, the trajectory of random walk is reflected by the boundary at a distance equal to the step  $h$  of approximation. Moreover, each such reflection introduces a bias in the estimator for the solution.

In this paper, we suggest a new approach to constructing statistical modeling methods, which makes it possible to use the algorithm of walk on spheres after the trajectory reaches the reflecting boundary. The approach is based on a new relation for the mean value of a function at a point belonging to the boundary rather than contained inside the domain, which makes it possible to substantially improve the performance of the stochastic computational algorithm.

## 2. INTEGRAL REPRESENTATION OF THE SOLUTION AT A BOUNDARY POINT

Let us construct a mean-value relation for the solution at a point  $x$  on the boundary of the domain. Without loss of generality, we can assume that  $x$  is an elliptic point. (This is always so if the trajectory of walk on spheres is constructed by the method of walk on subdomains [7].)

Consider the ball  $B(x, a)$  of radius  $a$  centered at the given point. Let  $\Phi_\kappa(y) = -\frac{1}{4\pi} \frac{\sinh(\kappa(a - |x - y|))}{|x - y| \sinh(\kappa a)}$  be

the Green function of the Dirichlet problem for Eq. (2) on the ball  $B(x, a)$  written for the central point  $x$ . Let us write the Green formula for the pair of functions  $u_i, \Phi_\kappa$  on  $B_i(x, a) \setminus B(x, \epsilon)$  and for the pair of functions  $u_e, \Phi_\kappa$  on  $B_e(x, a) \setminus B(x, \epsilon)$ . Here,  $B_i(x, a) = B(x, a) \cap G_i$ ,  $B_e(x, a) = B(x, a) \cap G_e$ , and  $S_i(x, a)$  and  $S_e(x, a)$  are, respectively, the interior and exterior parts of the surface of the sphere. In the obtained equalities, we pass to the limit as  $\epsilon \rightarrow 0$ , multiply them by  $\epsilon_i$  and  $\epsilon_e$ , respectively, and

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take the sum of the results. By virtue of the boundary conditions (3), we obtain

$$\begin{aligned}
 u(x) &= \frac{\epsilon_e}{\epsilon_e + \epsilon_i} \int_{S_e(x, a)} \frac{1}{2\pi a^2} \frac{\kappa a}{\sinh(\kappa a)} u_e ds \\
 &+ \frac{\epsilon_i}{\epsilon_e + \epsilon_i} \int_{S_i(x, a)} \frac{1}{2\pi a^2} \frac{\kappa a}{\sinh(\kappa a)} u_i ds \\
 &- \frac{\epsilon_e - \epsilon_i}{\epsilon_e + \epsilon_i} \int_{\Gamma \cap B(x, a) \setminus \{x\}} 2 \frac{\partial \Phi_0}{\partial n} Q_{\kappa, a} u ds \\
 &+ \frac{\epsilon_i}{\epsilon_e + \epsilon_i} \int_{B_i(x, a)} [-2\kappa^2 \Phi_\kappa] u_i dy \\
 &+ \frac{1}{\epsilon_e + \epsilon_i} \int_{B_i(x, a)} [-2\Phi_\kappa] \rho dy, \tag{4}
 \end{aligned}$$

where  $Q_{\kappa, a}(r) = \frac{\sinh(\kappa(a-r)) + \kappa r \cosh(\kappa(a-r))}{\sinh(\kappa a)} < 1$

and  $r = |x - y|$ . In the special case of  $\rho(x) = \sum_{m=1}^M q_m \delta(x - x_{c, m})$ , we assume that  $a < \min|x - x_{c, m}|$ , which ensures the absence of singularities inside the ball. As a consequence, the last integral in (4) vanishes.

In the limit case of  $\kappa = 0$ , this representation becomes simpler:

$$\begin{aligned}
 u(x) &= \frac{\epsilon_e}{\epsilon_e + \epsilon_i} \int_{S_e(x, a)} \frac{1}{2\pi a^2} u_e ds \\
 &+ \frac{\epsilon_i}{\epsilon_e + \epsilon_i} \int_{S_i(x, a)} \frac{1}{2\pi a^2} u_i ds \\
 &- \frac{\epsilon_e - \epsilon_i}{\epsilon_e + \epsilon_i} \int_{\Gamma \cap B(x, a) \setminus \{x\}} 2 \frac{\partial \Phi_0}{\partial n} u ds \\
 &+ \frac{1}{\epsilon_e + \epsilon_i} \int_{B_i(x, a)} [-2\Phi] \rho dy. \tag{5}
 \end{aligned}$$

Here,  $\Phi(y) = -\frac{1}{4\pi} \left( \frac{1}{|x-y|} - \frac{1}{a} \right)$  and  $2 \frac{\partial \Phi}{\partial n}(y) = \frac{1}{2\pi} \frac{\cos \phi_{yx}}{|x-y|^2}$ , where  $\phi_{yx}$  is the angle between the normal  $n(y)$  and the vector  $y - x$ . Note that if the boundary is plane, then  $\frac{\partial \Phi}{\partial n} = 0$  and, therefore, the integral over  $\Gamma$  is absent from the representation.

### 3. A STOCHASTIC COMPUTATIONAL ALGORITHM

Suppose that it is required to calculate the solution to problem (1)–(3) at a point  $x_0 \in G_i$ . We seek the solution in the form  $u(x) = u^0(x) + g(x)$ , where the potential

$g(x)$  equals  $\int_{G_i} \frac{1}{4\pi\epsilon_i|x-y|} \rho(y) dy$  or, in the case of point charges,  $\sum_{m=1}^M \frac{1}{4\pi\epsilon_i|x-x_{c, m}|} q_m$ . For the function  $u^0$ ,

which satisfies the Laplace equation on the bounded domain  $G_i$ , we construct an estimator being a functional of the trajectory of the Markov chain for walk on spheres:  $x_{i+1} = x_i + d(x_i)\omega_i$  [2]. Here,  $\{\omega_0, \omega_1, \dots\}$  is a sequence of independent unit isotropic vectors and  $d(x)$  is the distance from the point  $x$  to the boundary of the domain (or of the corresponding subdomain, if the method of walk on subdomains is used [7]). The Markov chain  $\{x_i, i = 0, 1, \dots\}$  converges to the boundary  $\Gamma$  with probability 1. Let  $x_k$  be the first point in the  $\epsilon$ -neighborhood [2] of  $\Gamma$ , and let  $x_k^* \in \Gamma$  be the point nearest to  $x_k$ . Obviously, the sequence  $u^0(x_i)$  is a martingale, and therefore  $u^0(x_0) = Eu^0(x_k) = E(u(x_k) - g(x_k)) = E(u(x_k^*) - g(x_k^*) + \phi)$ , where  $\phi = O(\epsilon)$  because of the assumption that the normal derivative exists at the point  $x_k^*$ .

To estimate the value of the solution at a boundary point, we use the mean relations obtained above. We regard the right-hand sides of these relations as an integral operator that transforms functions defined on the entire space into functions with domain  $\Gamma$ . The kernel of this operator may be alternating, and the convergence of the von Neumann series after replacing the kernel by its modulus cannot be ensured. As a consequence, the direct randomization of the integral equalities obtained above does not apply to constructing a Monte Carlo estimator [8], except if the boundary consists of planes.

Consider a simple probability approximation of the mean-value relation (5). Let us construct the tangent plane to the boundary at the point  $x_k^*$ . The next point  $x_{n+1}$  of the Markov chain is chosen uniformly on the hemisphere  $S^+(x_k^*, a)$  to which the normal vector is

directed with probability  $p_e = \frac{\epsilon_e}{\epsilon_i + \epsilon_e}$  and on the other

hemisphere  $S^-(x_k^*, a)$  with the complementary probability  $p_i$ . The value of the volume potential with density  $\rho$  is estimated at one random point, which is chosen with probability density depending on  $\Phi$ . Let  $\xi[I_\rho](x_k^*)$  be the estimate of this potential. Then, the following relation holds.

**Lemma 1.** As  $\frac{a}{2R} \rightarrow 0$ ,

$$E\{u(x_{k+1}) + \xi[I_\rho](x_k^*) | x_k^*\} = u(x_k^*) + O\left(\frac{a}{2R}\right)^3.$$

Here,  $R$  is the minimal radius of curvature of the surface  $\Gamma$  at the point  $x_k^*$ .

This assertion is easy to verify by direct integration. A similar assertion is valid when a given approximation is used to randomize relation (4). In this case, the coefficient under the sign of integral is treated as the survival probability for  $x_{k+1} \in S^+(x_k^*, a)$ . If the direction of the vector is chosen so that  $(x_{k+1} - x_k^*, n(x_k^*)) < 0$ , then the next point of the chain is taken on  $\frac{\kappa a}{\sinh(\kappa a)}$  with probability  $S^-(x_k^*, a)$  and in the corresponding half-ball with the complementary probability.

If  $x_{k+1} \in G_i$ , then we proceed to estimate the value of the function  $u^0$  at this point by the algorithm described above. In the case of exit to the exterior domain, we apply random walk on spheres. If  $\kappa = 0$ , then the modification with a direct modeling of the diffusion trajectory going to infinity is used [9]. If  $\kappa > 0$ ,

then the multiplier  $\frac{\kappa a}{\sinh(\kappa a)}$  in the mean-value formula for the Poisson–Boltzmann equation is treated as the survival probability, and the probability of the trajectory going to infinity vanishes.

An approximation of higher order of accuracy can be constructed by representing the integral operator in (4) as the difference  $K^+ - K^-$ . The kernel of  $K^+$  is positive, and this operator transforms functions defined on the sphere  $S(x, a)$  into functions on  $\Gamma \cap B(x, a)$ . Such a decomposition makes it possible to rewrite the integral relation (4) in the form  $u = (I + K^-)^{-1}K^+u$  and use it to construct more accurate approximations.

**Lemma 2.** The average number of boundary points in the Markov chain constructed above equals  $EN^* = \frac{2v}{a}(1 + dv)$ . here,  $v$  is a bounded solution to problem (1), (2) with boundary condition

$$\epsilon_i \frac{\partial v_i}{\partial n}(y) = \epsilon_e \frac{\partial v_e}{\partial n}(y) + 1,$$

and  $dv = O(a)$  as  $a \rightarrow 0$ .

This lemma follows from the fact that

$$\int_{\Gamma \cap B(x, a)} [-2\Phi] dy = \frac{a}{2} \text{ when } \Gamma \text{ is a plane or a sphere.}$$

Let  $\{x_{k,j}^* \in \Gamma, j = 1, 2, \dots, N_i^*\}$  be the sequence of points at which the constructed Markov chain exits from the domain  $G_i$  to the boundary, and let  $\{x_{k+1,j}^* \in$

$G_i, j = 1, 2, \dots, N_i^* - 1\}$  be the sequence of points at which it returns to this domain. Obviously,  $EN_i^* = p_i EN^*$ . Thus, the following assertion is valid.

**Statement.** The quantity

$$\begin{aligned} \xi[u](x_0) = & g(x_0) + \sum_{j=1}^{N_i^*-1} [\xi[I_\rho](x_{k,j}^*) - g(x_{k,j}^*) \\ & + g(x_{k+1,j}^*)] + \xi[I_\rho](x_{k,N_i^*}^*) - g(x_{k,N_i^*}^*) \end{aligned} \quad (6)$$

is an estimator for the solution to the boundary value problem (1), (2), (3). For  $\epsilon = \left(\frac{a}{2R}\right)^3$ , the bias of this estimator equals  $O(a^2)$  as  $a \rightarrow 0$ . The estimator has finite variance and complexity  $O(\ln(\delta) \cdot \delta^{-5/2})$  for a given accuracy  $\delta$ .

The variance is finite because the algorithm is based on a direct modeling [8] of the transformed integral equation. The estimate for complexity contains the logarithm because the mean number of transitions in the Markov chain of walk on spheres until the first entrance in the  $\epsilon$ -neighborhood of the boundary equals  $O(\ln(\epsilon))$  [2, 9]. The estimator  $\xi[\nabla u](x_0) = \nabla g(x_0) + Q_0 \xi[u_0](x_0)$  for the spatial derivatives is constructed for the same trajectories of walk on spheres as that for the solution. The weight  $Q_0$  is calculated at the first transition, in modeling an exit to the sphere  $S(x_0, d(x_0))$  [2].

Note that, when a finite-difference approximation with step  $h$  is used, the estimator has bias  $O(h)$  and complexity  $O(\ln(\delta) \cdot \delta^{-3})$  [4, 5]. Thus, even a simplest approximation of the integral equality constructed above makes it possible to substantially improve the efficiency of calculating the solution by the algorithm of walk on spheres.

#### 4. OTHER BOUNDARY VALUE PROBLEMS

Consider the practically important case where  $G_i$  and  $G_e$  are separated by an intermediate layer on which  $\kappa = 0$  and the coefficient of the Laplace operator equals  $\epsilon_e$ . On  $\partial G_i$  and  $\partial G_e$ , we have relations (5) and (4), respectively; from (4), both the boundary integral and volume potential are absent. All assertions about the algorithm based on the randomization of mean-value relations remain valid in this case.

The approach suggested in this paper applies to the exterior von Neumann problem virtually without changes. The situation with the mixed boundary value problem is somewhat more complicated. The radius  $a$  of the auxiliary sphere used to construct the integral relation may be arbitrarily small in this case. However, it can be shown that the probability of passing from the reflecting boundary to the absorbing boundary is always bounded away from zero. This implies that the algorithm has the same properties as in the case considered above. In solving the third boundary value prob-

lem, constructing approximations to the mean-value relation necessarily involves decomposing the integral operator and approximating the resolvent.

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