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A Feynman–Kac path-integral implementation for Poisson's equation using an *h*-conditioned Green's function

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Abstract

This study presents a Feynman–Kac path-integral implementation for solving the Dirichlet problem for Poisson's equation. The algorithm is a modified "walk on spheres" (WOS) that includes the Feynman–Kac path-integral contribution for the source term. In our approach, we use an *h*-conditioned Green's function instead of simulating Brownian trajectories in detail to implement this path-integral computation. The *h*-conditioned Green's function allows us to represent the integral of the right-hand-side function from the Poisson equation along Brownian paths as a volume integral with respect to a residence time density function: the *h*-conditioned Green's function. The *h*-conditioned Green's function allows us to solve the Poisson equation by simulating Brownian trajectories involving only large jumps, which is consistent with both WOS and our Green's function first-passage (GFFP) method [J. Comput. Phys. 174 (2001) 946]. As verification of the method, we tabulate the *h*-conditioned Green's function for Brownian motion starting at the center of the unit circle and making first-passage on the boundary of the circle, find an analytic expression fitting the *h*-conditioned Green's function, and provide results from a numerical experiment on a two-dimensional Poisson problem.

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Keywords: Walk on spheres; *h*-Conditioned Green's function; Poisson's equation

1. Introduction

Since Müller proposed the "walk on spheres" (WOS) method for solving the Dirichlet boundary value problems for the Laplace equation [2], WOS has been a popular method. In addition, this random-walk

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based approach has been extended to solve other, more complicated, partial differential equations including Poisson's equation, and the linearized Poisson–Boltzmann equation [3–9]. In WOS and our Green's function first-passage (GFFP) method [1], instead of using detailed Brownian trajectories inside the domain, discrete jumps are made using the first-passage probability distributions. In this paper, the WOS method, which utilizes the uniform first-passage probability distribution over a sphere, is combined with the Feynman–Kac formula to solve the Dirichlet boundary value problem for Poisson's equation. Even though the Feynman–Kac formula is well known among mathematicians and mathematical physicists, [10–12], as a computational technique, it has not been much implemented, even for simple cases, despite the fact that some modified WOS methods are mathematically derivable from Feynman–Kac [5]. We thus feel that it is worthwhile to present methods based on the Feynman–Kac formula for some simple problems to show its utility.

Here, we implement the Feynman–Kac formula for a simple Poisson problem. In the Feynman–Kac formula, the solution to a partial differential equation at a point is given as an average of a functional over Brownian motion trajectories. Instead of simulating the detailed Brownian trajectory, we use discrete WOS jumps together with an *h*-conditioned Green's function [11] to incorporate the source term in the Poisson equation. While different Green's functions have been used in previous work of others [3,5,9] for the source term in the Poisson's equation, the *h*-conditioned Green's function has never been used in this way. The *h*-conditioned Green's function gives the probability density distribution of a Brownian trajectory inside a ball during its passage from the ball's center to an exit point on the ball's boundary. It is a spherical analog of the Brownian bridge. This *h*-conditioned Green's function is used in place of a direct simulation of the Brownian trajectory because it gives the Brownian walker's density distribution inside the ball.

This paper is organized as follows. In Section 2, we explain how to implement the Feynman–Kac path-integral method for the Dirichlet problem for Poisson's equation. In Section 3, we give a numerical example. In Section 4, conclusions are presented and future work is discussed.

2. Modified "walk on spheres"

In this section, we explain how to combine the WOS method [2] with the Feynman–Kac path-integral representation for solving the Dirichlet problem for Poisson's equation. Our implementation is based on the well-known Feynman–Kac representation of the solution to the Dirichlet problem for Poisson's equation. Recall that the Dirichlet problem for Poisson's equation is:

$$\tfrac{1}{2}\Delta u(\boldsymbol{x}) = -q(\boldsymbol{x}), \quad \boldsymbol{x} \in D, \tag{1}$$

$$u(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial D. \tag{2}$$

The solution to this problem at the point $\boldsymbol{x}_0$, given in the form of the path-integral with respect to standard Brownian motion W_t, is as follows [10,11]:

$$u(\boldsymbol{x}_0) = E\left[\int_0^{\tau_{\partial D}} q(W_t)\,\mathrm{d}t\right] + E[f(W_{\tau_{\partial D}})]. \tag{3}$$

Here, $\tau_{\partial D} = \inf\{t : W_t \in \partial D\}$ is the first-passage time and $W_{\tau_{\partial D}}$ is the first-passage location on the boundary, ∂D. Here, we assume that $E[\tau_{\partial D}] < \infty$ for all $\boldsymbol{x}_0 \in D$, $f(\boldsymbol{x})$ and $q(\boldsymbol{x})$ are continuous and

bounded, and that the boundary, ∂D, is sufficiently smooth so as to ensure the existence of a unique solution, $u(\boldsymbol{x})$, that has bounded and continuous first- and second-order partial derivatives in any interior subdomain [10,11].

Instead of simulating the detailed irregular motion of the Brownian trajectories, we use the *h*-conditioned Green's function [11] for a ball with WOS as a probability density function. The *h*-conditioned Green's function gives the probability density distribution of the Brownian trajectory inside the ball during its passage from the center to the boundary. We construct a Brownian trajectory as a sequence of discrete jumps from ball centers to ball surfaces. By using the *h*-conditioned Green's function, $K(\boldsymbol{x}, \boldsymbol{z})$, the first term of Eq. (3) for the ith ball of a WOS (Brownian) trajectory becomes [11]:

$$\int_{B_i} q(\boldsymbol{x}) K(\boldsymbol{x}, \boldsymbol{z})\, \mathrm{d}\boldsymbol{x}. \tag{4}$$

Here, B_i is the ith ball and $\boldsymbol{z}$ is the first-passage location on the surface of the ball, making the preceding a volume integral.

Eq. (4) readily permits the use of WOS to eliminate the need to compute the detailed Brownian trajectory. Instead, the Brownian trajectory is built up with a series of discrete jumps in continuous space terminating on the boundary, ∂D. Jumping from ball to ball never permits a trajectory to land exactly on the boundary. Thus, we use the standard WOS approach of "fattening" the boundary by ϵ to create a capture region that is used to terminate the walk [3]. The error associated with this approximation has been theoretically estimated in previous WOS studies [7,9] and with our GFFP method no ϵ-absorption layer is needed [1].

We wish to compute the solution to the Dirichlet problem for Poisson's equation at $\boldsymbol{x}_0$. For each Brownian trajectory starting at $\boldsymbol{x}_0$, with an ϵ-absorption layer, we accumulate the internal contribution for each ball and score the functional value of the boundary condition at the final exit location on ∂D. And so, an estimate for the solution at $\boldsymbol{x}_0$ is given by the statistic

$$S_N = \frac{1}{N} \sum_{i=1}^{N} Y_i, \tag{5}$$

where N is the number of trajectories and each statistic, Y_i, is given by

$$Y_i = \sum_{j=1}^{n_i} \left[\int_{B(\boldsymbol{x}_j^i, r_j^i)} q(\boldsymbol{x}) K^i(\boldsymbol{x}, \boldsymbol{z}_j^i)\, \mathrm{d}\boldsymbol{x} \right] + f(W_{\tau_{\partial D}^i}). \tag{6}$$

Here, n_i is the number of WOS steps needed for the ith Brownian trajectory to terminate in the ϵ-absorption layer, $\boldsymbol{x}_j^i$ is the center of the jth ball of radius r_j^i, $\boldsymbol{z}_j^i$ the first-passage location on the surface of the jth ball, and $W_{\tau_{\partial D}^i}$ is the first-passage location on the boundary, ∂D.

3. Numerical experiments

In this section, we demonstrate our Feynman–Kac implementation by solving numerically a boundary value problem for Poisson's equation. We use as our domain, D, the unit disk minus the first quadrant, which was used in previous research by DeLaurentis and Romero [9] (See Fig. 1).

We consider the Poisson equation:

$$\tfrac{1}{2}\Delta u(\boldsymbol{x}) = -\left(1 - \tfrac{1}{2}r^2\right) \mathrm{e}^{-r^2/2} \tag{7}$$

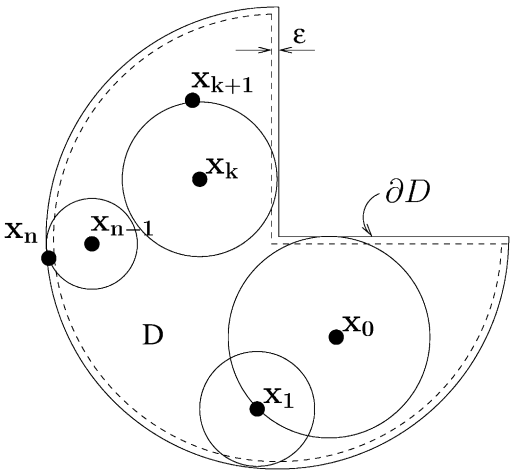

Fig. 1. Modified WOS: $\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_k, \ldots, \boldsymbol{x}_n$ are a series of discrete jumps of a Brownian trajectory which terminates on absorption in the ϵ-absorption layer.

with the boundary conditions $u(r, 0) = \mathrm{e}^{-r^2/2}$, $u(r, -3\pi/2) = -r^{1/3} + \mathrm{e}^{-r^2/2}$, and $u(1, \theta) = \sin(\theta/3) + \mathrm{e}^{-1/2}$. The known analytic solution is

$$u(r, \theta) = r^{1/3} \sin\left(\tfrac{1}{3}\theta\right) + \mathrm{e}^{-r^2/2}. \tag{8}$$

For this two-dimensional problem, the *h*-conditioned Green's function was obtained via simulation at first and later found in analytic form (see Appendix A). The cumulative radial distribution, $\rho(r)$, on the unit circle of this *h*-conditioned Green's function is given by

$$\rho(r) = r^2(2\log(r) + 1), \tag{9}$$

and the conditional cumulative angular distribution, $\rho(\phi)$, by

$$\rho(\phi) = \frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{1+a}{1-a}\tan\left(\frac{\phi}{2}\right)\right). \tag{10}$$

Here, a is the given radial position and ϕ ranges from $-\pi$ to π with respect to the first-passage location on the circular boundary. In Fig. 2, the cumulative density functions are shown. The simulation to compute the *h*-conditioned Green's function was done on the unit circle with 10^4 Brownian trajectories, a 10^{-4} sized ϵ-absorption layer, and radial step size of 0.012 (see Fig. 3). For each Brownian trajectory, we record the locations of the Brownian trajectory at each step until first-passage on the circular boundary. After each trajectory, we rotate this distribution to the reference first-passage location and accumulate the results. This method is what we refer to as the simulation–tabulation method [1]. It should be noted that the cumulative radial distribution found here is the same as that used previously by other researchers [9], and the analytic form of the conditional cumulative angular distribution is the two-dimensional Poisson kernel [11].

The *i*th estimate of the solution to Poisson's equation is given by

$$Y_i = \sum_{j=1}^{n_i} \left[\int_{B(\boldsymbol{x}_j^i, r_j^i)} q(\boldsymbol{x}) K^i(\boldsymbol{x}, \boldsymbol{z}_j^i)\, \mathrm{d}\boldsymbol{x} \right] + f(W_{\tau_{\partial D}^i}). \tag{11}$$

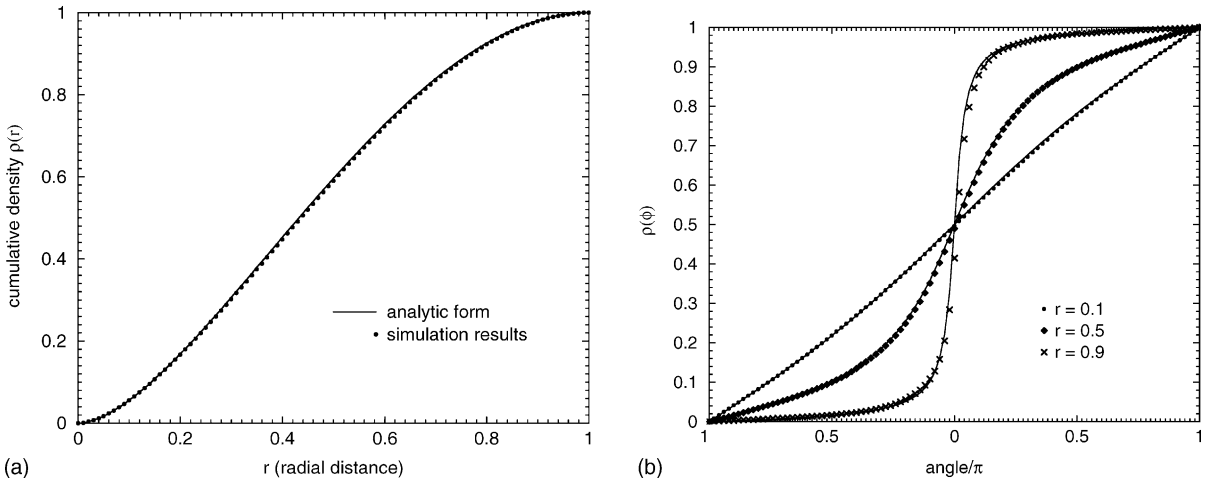

Fig. 2. *h*-Conditioned Green's function. (a) Cumulative radial distribution, $\rho(r)$, on the unit circle: the filled circles are the simulation results and the solid line is the analytic form. (b) Conditional cumulative angular distribution, $\rho(\phi)$, on the unit circle: the filled circles, diamonds and crosses are the simulation results and the solid lines are the analytic forms. The angle is with respect to the first-passage location on the circular boundary.

Here, $\boldsymbol{x}_j^i$ is the center of the circle of radius r_j^i. Instead of integrating the first term of Eq. (11), we can use the "one-point random estimation inside the sphere" (OPRE) method [9]:

$$Y_i = \sum_{j=1}^{n_i} \tfrac{1}{4}(r_j^i)^2 E[q(C_j^i)] + f(W_{\tau_{\partial D}^i}). \tag{12}$$

Here, C_j^i is the sampling location inside the jth circle. At first, the radial position is selected according to the cumulative radial density and for the given radial position the angular position is selected according

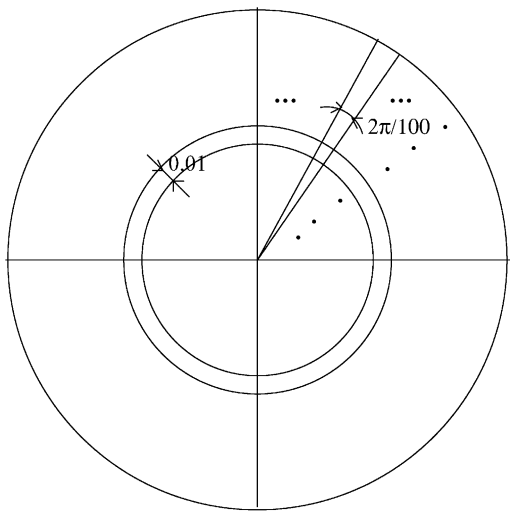

Fig. 3. Simulation on the unit circle: the radial and angular positions are divided into 100 grid points.

Table 1
Simulation results for the solution at five different points

r	θ	Exact	Monte Carlo	Variance	Average number of steps
0.1244	−0.7906	0.8623	0.8605	0.0948	19.67
0.2320	−0.0274	0.9678	0.9677	0.0049	15.48
0.2187	−3.3975	0.4308	0.4295	0.1797	20.52
0.1476	−4.1617	0.4696	0.4688	0.0848	19.25
0.0129	−1.4790	0.8889	0.8889	0.0555	18.81

The absorption layer thickness is $\epsilon = 10^{-6}$ and the number of trajectories $N = 10^5$.

to 2 arctan$[\{(1-x)/(1+x)\}\tan(\pi\eta)]$, where η is a random number uniform in $(-0.5, 0.5)$. The angular position ranges from $-\pi$ to π with respect to the first-passage location on the circular boundary. Table 1 shows our simulation results for the solution at five different points. The absorption layer thickness is $\epsilon = 10^{-6}$, and the number of trajectories for each run is $N = 10^5$.

The errors associated with this implementation are (1) the error associated with the number of trajectories (sampling error), (2) the error associated with the ϵ-absorption layer, and (3) the error associated with the integration used for the source term. We can reduce the statistical sampling error by increasing the number of trajectories. The error associated with the ϵ-absorption layer can be reduced by reducing ϵ, the ϵ-absorption layer thickness. However, increasing the number of trajectories will increase the running time linearly, while reducing ϵ will increase running time as $O(|\log\epsilon|)$. In Fig. 4(a), we see the usual relationship between running time and the thickness of the ϵ-absorption layer in WOS: $O(|\log\epsilon|)$. The reason for this is that the running time increases proportionally to the number of WOS steps, n_i, which is itself $O(|\log\epsilon|)$ [3]. The error from the ϵ-absorption layer can be investigated empirically if we have enough trajectories so that the statistical sampling error is much smaller than the error from the ϵ-absorption layer [13]. Fig. 4 (b) shows the empirical results with 10^7 Brownian trajectories: the ϵ-layer

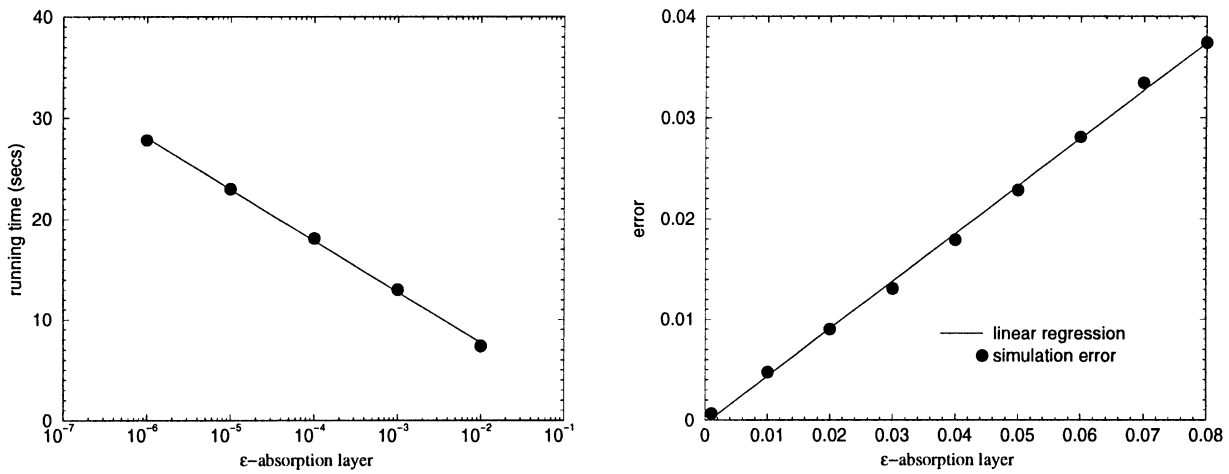

Fig. 4. (a) Running time vs. the thickness of the ϵ-absorption layer with 10^5 Brownian trajectories. This shows the usual relation for WOS, running time (proportional to number of WOS steps for each Brownian trajectory) $O(|\log\epsilon|)$. (b) Absolute error arising from the ϵ-absorption layer with 10^7 Brownian trajectories in the case of the first row in Table 1. The error is linear in ϵ.

error grows linearly in ϵ for small ϵ. Instead of direct integration, we use OPRE method. However, if the source term has much variation the OPRE method may not be so efficient. More points might have to be used in the areas where variation is big [3]. If we use faster integration subroutine or quardruture rule, it may be better to use the direct integration for the source term than OPRE inside the circle.

4. Conclusions and future work

In this study, we implemented the Feynman–Kac path-integral representation of the solution to the Dirichlet problem for Poisson's equation combining the well known WOS method with use of the *h*-conditioned Green's function. Using the *h*-conditioned Green's function inside each WOS step, we avoid the need for detailed information about the Brownian trajectory inside the spherical domain. The Brownian trajectory is thus constructed as a series of discrete jumps using WOS with the source contribution inside each WOS step computed using the *h*-conditioned Green's function. The *h*-conditioned Green's function is obtained via simulation in two dimensions at first and later it turns out that the *h*-conditioned Green's function is the combination of the usual angle-averaged Green function [9] for the radial distribution and the Poisson kernel [11] for the angular distribution.

Recently, we developed a modified WOS algorithm for solving the linearized Poisson–Boltzmann equation [8] in a domain D:

$$\Delta\psi(\boldsymbol{x}) = \kappa^2\psi(\boldsymbol{x}), \quad \boldsymbol{x} \in D, \tag{13}$$

$$\psi(\boldsymbol{x}) = \psi_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial D. \tag{14}$$

Here, κ is called the inverse Debye length [14]. We used a survival probability, which was obtained by reinterpreting a weight function in a previously modified WOS method [5]. This survival probability enabled us to terminate some Brownian trajectories during WOS steps. This method can be combined with the method described in this paper to solve the Dirichlet boundary value problem for $\Delta\psi(\boldsymbol{x}) - \kappa^2\psi(\boldsymbol{x}) = -g(\boldsymbol{x})$. This will be the subject of a future study.

Also, it should be noted that the Feynman–Kac path-integral representation is general and the *h*-conditioned Green's function can be obtained for any geometry via simulation. This opens up the possibility of removing the ϵ-absorption layer in WOS methods and extending the *h*-conditioned Green's function to the GFFP method. In three dimensions, we can also obtain the *h*-conditioned Green's function for a sphere using the Poisson kernel in three dimensions and the (angle-averaged) Green's function.

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Appendix A

In this appendix, we show the relation of the conditional cumulative angular distribution of the *h*-conditioned Green's function to the Poisson kernel. Let us start with the Dirichlet problem for the

unit disk using polar coordinates:

$$\Delta u(r,\theta) = 0, \quad \boldsymbol{x} \in D, \tag{A.1}$$

$$u(1,\theta) = f(\theta), \quad \boldsymbol{x} \in \partial D. \tag{A.2}$$

The solution to this problem is given by [15]

$$u(r,\theta) = \int_0^{2\pi} P(r,\theta,\phi) f(\phi)\, \mathrm{d}\phi, \quad r < 1, \tag{A.3}$$

$$u(1,\theta) = f(\theta), \tag{A.4}$$

where the Poisson kernel, $P(r,\theta,\phi)$, is

$$P(r,\theta,\phi) = \frac{1}{2\pi} \frac{1-r^2}{(1+r^2-2r\,\cos(\theta-\phi))}. \tag{A.5}$$

For the conditional cumulative angular distribution of the *h*-conditioned Green's function, we use the condition at the first-passage point on the boundary

$$u(1,\theta) = \delta(\theta-\theta_1), \tag{A.6}$$

where θ_1 is the angle of the first-passage point. Then the solution to this Dirichlet boundary problem becomes the Poisson kernel:

$$u(r,\theta) = \frac{1}{2\pi} \frac{1-r^2}{(1+r^2-2r\,\cos(\theta-\theta_1))}, \quad r < 1, \tag{A.7}$$

$$u(1,\theta) = \delta(\theta-\theta_1). \tag{A.8}$$

If we integrate the Poisson kernel from $-\pi$ to ϕ, for simplicity, with $\theta_1 = 0$ and normalize, we get the conditional cumulative angular distribution function.

References

[1] C.-O. Hwang, J.A. Given, M. Mascagni, The simulation–tabulation method for classical diffusion Monte Carlo, J. Comput. Phys. 174 (2) (2001) 925–946.
[2] M.E. Müller, Some continuous Monte Carlo methods for the Dirichlet problem, Ann. Math. Stat. 27 (1956) 569–589.
[3] K.K. Sabelfeld, Monte Carlo Methods in Boundary Value Problems, Springer, Berlin, 1991.
[4] A. Haji-Sheikh, E.M. Sparrow, The solution of heat conduction problems by probability methods, J. Heat Transfer 89 (1967) 121–131.
[5] B.S. Elepov, G.A. Mihailov, The "walk on spheres" algorithm for the equation $\delta u - cu = -g$, Sov. Math. Dokl. 14 (1973) 1276–1280.
[6] T.E. Booth, Exact Monte Carlo solution of elliptic partial differential equations, J. Comput. Phys. 39 (1981) 396–404.
[7] T.E. Booth, Regional Monte Carlo solution of elliptic partial differential equations, J. Comput. Phys. 47 (1982) 281–290.
[8] C.-O. Hwang, M. Mascagni, Efficient modified "walk on spheres" algorithm for the linearized Poisson–Boltzmann equation, Appl. Phys. Lett. 78 (6) (2001) 787–789.
[9] J.M. De Laurentis, L.A. Romero, A Monte Carlo method for Poisson's equation, J. Comput. Phys. 90 (1990) 123–139.
[10] M. Freidlin, Functional Integration and Partial Differential Equations, Princeton University Press, Princeton, NJ, 1985.
[11] K.L. Chung, Z. Zhao, From Brownian Motion to Schrödinger's Equation, Springer, Berlin, 1995.

[12] K.K. Sabelfeld, Integral and probabilistic representations for systems of elliptic equations, Math. Comput. Modell. 23 (1996) 111–129.
[13] M. Mascagni, C.-O. Hwang, ϵ-Shell error analysis in "walk on spheres" algorithms, Math. Comput. Simulat., 2001, submitted for publication.
[14] R. Ettelaie, Solutions of the linearized Poisson–Boltzmann equation through the use of random-walk simulation method, J. Chem. Phys. 103 (9) (1995) 3657–3667.
[15] E.C. Zachmanoglou, D.W. Thoe, Introduction to Partial Differential Equations with Applications, Dover, New York, 1976.