Edge distribution method for solving elliptic boundary value problems with boundary singularities

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Elliptic boundary value problems are difficult to treat in the vicinity of singularities, i.e., edges and corners, of the boundary. The concentration of electrical charge on the edges and corners of a conductor is perhaps the simplest example of such problems. Here we provide a rapid method for accurate treatment of these problems. It utilizes a Green's-function-based implementation of last-passage Monte Carlo diffusion methods. This is combined with a diffusion algorithm for the scaling of solutions to the Laplace equation near a corner singularity to yield the solution of a benchmark problem: the charge distribution near the edge and corner of a conducting cube.

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I. INTRODUCTION

Probabilistic potential theory [1,2] allows the accurate solution of elliptic partial differential equations (PDE's) using methods naturally suited to parallel programming. Thus it shows promise as a source of computational methods for application domains in which numerically intensive problems of this kind must be solved. In the present research, we restrict our study to the Laplace and Poisson equations. Two important application areas are the calculation of molecular potentials in protein biophysics [3–5] and the calculation of permeabilities of samples of porous media [6–8].

This paper is a contribution to a project of solving these problems using a class of ''charge-based'' methods, i.e., methods that focus on calculating the surface charge, i.e., the normal gradient of the solution at all surfaces on which boundary conditions are imposed. From this information, one can reconstruct the solution at an arbitrary point, using, e.g., the method of moments [9].

The set of methods developed or extended within this project includes walk on spheres (WOS) method [10,11], first-passage methods [3,12–14], Green's function first-passage methods [7,15,16] (good for problems with very irregular boundaries), and last-passage methods [17,18], in which diffusing particles are created at the site where they are to be absorbed, and carry out time-reversed Brownian motion (good for multiabsorber problems, and for problems in which surface charge is highly concentrated in a nonuniform manner).

The first-passage method generates a surface charge distribution, one charge at a time: each diffusing particle initiates outside the conducting surface, diffuses until it first reaches the surfaces, and is absorbed, leaving a unit charge at the contact point.

By contrast, the last-passage method uses an integral formula for the surface charge density to calculate this quantity at a discrete set of points, e.g., the points chosen by an adaptive integration algorithm, to calculate the total charge on the surface. Alternatively, the charge density can be calculated on a uniform two-dimensional mesh, the entire surface charge distribution being obtained by interpolating the points using quadratic splines.

It is difficult to use probabilistic potential theory to obtain the surface charge density at any point with high accuracy: The law of large numbers shows that a quantity defined by the sum of N independent, random contributions has a width in distribution that is proportional to $1/\sqrt{N}$. In problems for which the surface charge distribution is smooth, this slow convergence can be overcome by calculating, from the same Brownian paths that provide $\sigma(x)$, the matrix of partial derivatives of this quantity. One then obtains the quantity $\sigma(x)$ with high accuracy by using a stochastic version of Taylor's theorem [19]. In problems for which the boundary contains singularities (edges and corners), this process must be augmented; this is the basic purpose of this paper.

In the most basic elliptic PDE, the surface charge, i.e., the gradient of the solution, is concentrated near singularities (edges and corners) of the boundary. The calculation of the charge singularity at a generalized corner, a meeting point for three or more boundary surfaces, is very demanding when standard applied math techniques are used. Among methods currently being applied to the study of boundary singularities are the multipole method [20], boundary element method extrapolation [21,22], and the use of singular basis functions in the Galerkin method [23].

In this paper we present a method for obtaining the behavior of charge distributions near surface singularities, and using that information to obtain the function $\sigma(x)$ over the entire surface. We call this method the edge distribution (ED) method.

The basic idea of the ED method is the following: a large fraction of the total surface charge is found near the corners and edges. But this fraction is difficult to calculate with the last-passage methods just described, because mesh integration algorithms converge slowly when applied to rapidly varying functions. The surface charge density at points near an edge can be written

$$\sigma(\mathbf{x},\delta) = \delta^{\pi/\alpha - 1}\sigma_e(\mathbf{x}), \tag{1}$$

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where δ is the distance from the edge and α is the exterior angle between the two intersecting surfaces that form the edge, i.e., it is the angle as swept out through space external to the conductor (see Fig. 2.) Here the edge distribution $\sigma_e(\mathbf{x})$ is defined by the fact that it is independent of δ for small δ. The charge density at all points near to an edge is completely determined by its edge distribution $\sigma_e(x)$. This quantity needs to be calculated only once for each geometrically distinct edge in a problem. In this paper, we provide an efficient last-passage method for calculating the function $\sigma_e(\mathbf{x})$. For conductors of high symmetry, such as those treated here, the edge distribution is best obtained by using the simulation-tabulation method [16].

In this paper, we introduce the edge distribution method as an important extension of last-passage methods. We demonstrate its value by calculating the charge distribution near the edges and corners of a cubic conductor.

An additional result of this study is to provide a rapid, accurate method of exploring corner singularities. The charge density near a corner of a conductor is known to become singular as a power of the distance from the corner. Here we restrict our study to corners formed by three locally planar surfaces; even in this case, the exponent of the singularity is known to depend on the geometry of the corner.

Existing numerical methods for determining this singularity require the use of specialized eigenfunction expansions [24–27]. Here we show that probabilistic potential theory provides a simple, general solution to this class of problems.

This paper is organized as follows: in Sec. II, we review the last-passage method for the charge density on a conducting surface held at unit voltage. In Sec. III, we develop the ED method for fast calculation of charge density near the edges of a conductor. In Sec. IV, the ED method is applied to calculate the charge distribution near the edges and corners of a basic test case: the conducting cube. Discussions and conclusions are contained in Sec. V.

II. THE LAST-PASSAGE ALGORITHM AND ITS LIMITATIONS

In this section, we review the last-passage method for charge density on a conducting surface held at unit voltage with respect to infinity and note some difficulties associated with the method [18].

First, we review the last-passage method for charge density on a conducting surface held at unit voltage with respect to infinity. The last-passage algorithm for charge density relies on the basic isomorphism of probabilistic potential theory [1,2]. We briefly review this isomorphism.

Consider the potential $\Phi(\mathbf{x})$ at a point $\mathbf{x}$ near a set of conducting surfaces. This quantity is closely related [18,20] to the probability $P(\mathbf{x})$ that a diffusing particle initiates at the point $\mathbf{x}$ and executes Brownian motion in an environment of absorbing surfaces whose geometry is identical to the set of conducting surfaces, and diffuses very far away without ever being absorbed at any of these surfaces. [To be precise, one has $P(\mathbf{x})=1-\Phi(\mathbf{x})$.] This formula is of central importance in the solution of Laplace (and related) equations; it allows one to express the solutions of these equations as weighted averages over the properties of Brownian paths.

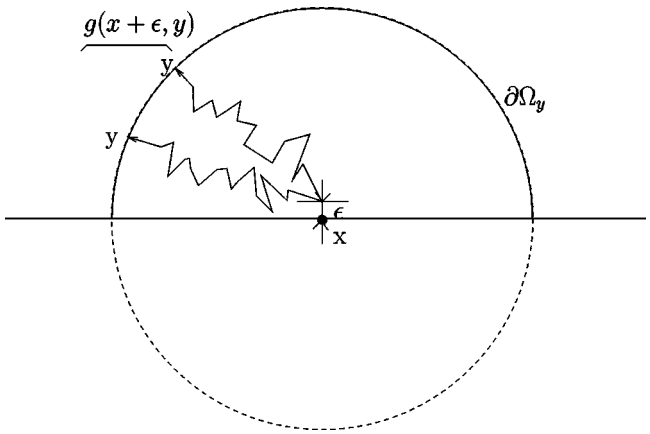

FIG. 1. A conducting surface is shown edge on. $g(\mathbf{x}+\boldsymbol{\epsilon},\mathbf{y})$ is the Laplace Green's function, i.e., it gives the probability density associated with a diffusing particle initiating at the point $\mathbf{x}+\boldsymbol{\epsilon}$ and making first passage on the surface $\partial\Omega_y$ at the point $\mathbf{y}$. For small $\boldsymbol{\epsilon}$, the distribution of walkers leaving the point $(x+\boldsymbol{\epsilon})$ and not touching the horizontal surface can be written $\boldsymbol{\epsilon}\overline{g}(x,y)$.

This isomorphism, together with basic probability theory, yields a formula for the surface charge density $\sigma(\mathbf{x})$ at a point on a boundary of a conducting object. Because $P(x)$ is a harmonic function, it obeys the following equation:

$$P(\mathbf{x}+\boldsymbol{\epsilon})=\int d\Omega_y\, g(\mathbf{x}+\boldsymbol{\epsilon},\mathbf{y})P(y). \tag{2}$$

Here, $g(\mathbf{x}+\boldsymbol{\epsilon},\mathbf{y})$ is the Laplacian Green's function associated with Dirichlet, or absorbing, boundary conditions on the surface $\partial\Omega$ of the closed region Ω_y surrounding the point x (see Fig. 1). In probabilistic language, $g(\mathbf{x}+\boldsymbol{\epsilon},\mathbf{y})$ is the probability density associated with finding a diffusing particle leaving point $\mathbf{x}+\boldsymbol{\epsilon}$ and making first passage at the point $\mathbf{y}$ on a surface surrounding the point $\mathbf{x}+\boldsymbol{\epsilon}$. Equation (2) expresses the mean-value theorem for the harmonic function $P(x)$: in order to leave point x and diffuse far away, a diffusing particle must leave point x and make first passage at a point y [28]. It must then leave point y and diffuse far away. Note that, for small $\boldsymbol{\epsilon}$, the first factor in the integrand is proportional to $\boldsymbol{\epsilon}$; the second factor becomes $\boldsymbol{\epsilon}$ independent. The charge density at the point $\mathbf{x}$ is given by Gauss's law [29] as

$$\sigma(\mathbf{x})=-\frac{1}{4\pi}\frac{d}{d\boldsymbol{\epsilon}}\bigg|_{\boldsymbol{\epsilon}=0}\Phi(\mathbf{x}). \tag{3}$$

Using the isomorphism of the probability $P(\mathbf{x})$ to the electrostatic potential $\Phi(\mathbf{x})$ gives

$$\sigma(\mathbf{x})=\frac{1}{4\pi}\frac{d}{d\boldsymbol{\epsilon}}\bigg|_{\boldsymbol{\epsilon}=0}P(\mathbf{x}+\boldsymbol{\epsilon}). \tag{4}$$

Substituting Eq. (2) gives

$$\sigma(\mathbf{x})=\frac{1}{4\pi}\int d\boldsymbol{\Omega}_{\mathbf{y}}\,\overline{g}(\mathbf{x},\mathbf{y})P(y). \tag{5}$$

Here,

$$\overline{g}(\mathbf{x},\mathbf{y}) \equiv \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} g(\mathbf{x}+\epsilon,\mathbf{y}). \tag{6}$$

This equation provides a factorization which is valuable for calculating $\sigma(\mathbf{x})$ on a conducting surface: the function $\overline{g}(\mathbf{x},\mathbf{y})$ can be treated analytically. The function $P(\mathbf{y})$ is complicated, but it can be obtained by Monte Carlo simulation using the Green's-function first-passage (GFFP) method [7,8,16,17].

The function $\overline{g}(x,y)$ is a point-dipole Green's function; it gives the solution to the Laplace Dirichlet problem for a conducting surface surrounding a point dipole at position $\mathbf{x}$. The above derivation shows that, in the case where the point $\mathbf{x}$ lies on a different conducting surface, the function $\overline{g}(\mathbf{x},\mathbf{y})$ is also a last-passage Green's function, i.e., it gives the probability density associated with a Brownian particle leaving an absorbing surface at point $\mathbf{x}$ and diffusing to point $\mathbf{y}$ without ever returning to that surface.

The function $\overline{g}(\mathbf{x},\mathbf{y})$ has been obtained analytically for a point dipole oriented normal to a flat conducting surface [18]:

$$\overline{g}(x,y) = \frac{3}{2\pi} \frac{|xy|}{|x||y|} \frac{1}{|x-y|^3} = \frac{3}{2\pi} \frac{\cos\theta}{d^3}, \tag{7}$$

where θ is the polar angle and d the radius of the absorbing half sphere. Thus, the charge density on a flat surface of a conducting object is given by

$$\sigma(\mathbf{x}) = \frac{3}{8\pi^2} \int d\Omega_y \frac{\cos\theta}{d^3} P(\mathbf{y}). \tag{8}$$

This formula is the basis for a last-passage Monte Carlo algorithm for the charge density in the problem studied here: diffusing particles are placed at random points $\mathbf{y}$ on a first-passage sphere surrounding the point $\mathbf{x}$, according to the probability distribution $\overline{g}(x,y)$. The GFFP method [7,8,16,17] is then used to simulate the diffusion of these particles. If a diffusing particle fails to return to the conducting surface containing the point $\mathbf{x}$, the random variable $P(\mathbf{x})$ takes on the value unity for this diffusion trial; these diffusing particles will contribute to the Monte Carlo evaluation of the right-hand side of Eq. (8).

The last-passage method is inaccurate in evaluating the charge density for points $\mathbf{x}$ very near the edges and corners of a conducting object. The charge density $\sigma(\mathbf{x})$ tends to be large; the first factor in the integrand of Eq. (5) tends to be very large and the second factor tends to be very small (the last two essentially because the radius of the hemisphere d must be chosen very small for points x very near the edge). Thus statistical errors can be very large. Next, we address this problem.

III. THE EDGE DISTRIBUTION METHOD

In this section, we introduce a technique, the edge distribution method, that extends the validity of the last-passage method to the boundary of the region containing singularities. For any edge of a conducting surface, the charge distribution $\sigma(\mathbf{x},\delta)$ on a curve parallel to the edge, but separated from it by distance δ, with δ small, can be expressed as

$$\sigma(\mathbf{x},\delta) = \delta^{\pi/\alpha - 1} \sigma_e(\mathbf{x}). \tag{9}$$

Here the edge distribution $\sigma_e(\mathbf{x})$ is nonsingular as δ goes to zero; the angle α is the angle between the two surfaces whose intersection forms the edge; see Fig. 2. The edge distribution has a natural probabilistic interpretation: it is the (rescaled) probability density that a diffusing particle makes last passage on the edge point x. According to the discussion of the last section, it is also the (rescaled) charge distribution on a conductor of the same size and shape.

Once one has both the basic scaling law, Eq. (9), and the edge distribution for each edge, one can quickly calculate all the charge near edges and corners. The point is that this one-dimensional distribution needs to be determined only once for each edge on each absorbing object in a calculation.

For each $\mathbf{x}$ value of interest, one can calculate the edge distribution using the following formula:

$$\sigma_e(\mathbf{x}) = \lim_{\delta \to 0} \delta^{1-\pi/\alpha} \sigma(\mathbf{x},\delta), \tag{10}$$

where $\sigma(\mathbf{x},\delta)$ gives the surface charge density along a line, located on one of the two intersecting surfaces, which is parallel to the edge but a distance δ away from it. The limit in this formula is evaluated by obtaining the quantity $\sigma(\mathbf{x},\delta)$ for two or three small values of δ, and then extrapolating to $\delta=0$. This last quantity is obtained by simulation using the last-passage formula, Eq. (8).

In the cases we study in this paper, the function $\sigma_e(\mathbf{x})$ can be obtained as follows: first we substitute for $\sigma(x,\delta)$ a form of the integral expression, Eq. (8). It is necessary to choose an appropriate form of the Dirichlet Green's function $g(x,y)$. Because we treat the region near the intersection of two planar, absorbing surfaces, we choose a Green's function corresponding to a first-passage surface which is a chopped cylinder, whose central axis contains the edge in question (see Fig. 2). This Green's function can be obtained analytically as an infinite series. The surface charge is obtained by taking a normal derivative of the function $g(x,y)$, at each conducting surface, to give $\overline{g}(x,y)$. Finally, the limit $\delta \to 0$ in Eq. (10) can be taken analytically. The resulting formula is the basis for a diffusion Monte Carlo calculation of the edge distribution (see Fig. 3).

We describe in detail the calculation of the edge distribution Green's function for the geometry of the cube, i.e., for a pair of planar conducting surfaces meeting at an angle of $\alpha = 3\pi/2$.

The geometry associated with the edge distribution Green's function in the case of a cube is shown in Fig. 2. The diffusing particle begins at a point x on the edge of the cube. It is surrounded by a first-passage surface which is a three-quarter cylinder of length L and radius a. It is the portion of a cylinder, with centerline given by the edge, that is outside the absorbing cube. The potential inside the three-quarter

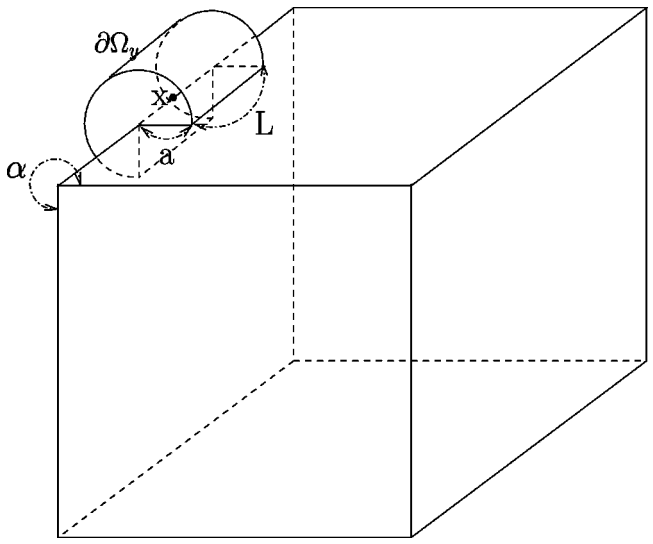

FIG. 2. The cylindrical first-passage surface of radius a and length L centered on the edge of a cube. Here $\partial\Omega_y$ is a chopped cylindrical surface that intersects the pair of absorbing surfaces meeting at angle $\alpha=3\pi/2$.

cylinder at a point whose cylindrical coordinates are (ρ,ϕ,z) due to a charge at position (ρ',ϕ',z') is obtained as [29]

$$\Phi(\rho,\phi,z)=\frac{4}{L}\sum_{n=1}^{\infty}\sin\left(\frac{2}{3}\phi\right)\sin\left(\frac{2}{3}\phi'\right)\sin\left(\frac{n\pi z}{L}\right)\times\sin\left(\frac{n\pi z'}{L}\right)\frac{I_{2/3}(n\pi\rho'/L)}{I_{2/3}(n\pi a/L)}\left[I_{2/3}\left(\frac{n\pi a}{L}\right)\times K_{2/3}\left(\frac{n\pi\rho}{L}\right)-K_{2/3}\left(\frac{n\pi a}{L}\right)I_{2/3}\left(\frac{n\pi\rho}{L}\right)\right]. \tag{11}$$

Here we assume that $\rho'<\rho$. Also, $I_{2/3}$ and $K_{2/3}$ are modified Bessel functions of the first and second kinds, respectively, of order two-thirds. From the above potential, we can get the charge density distribution $g(\rho,\phi,z)$ [29].

The last-passage Green's function $\overline{g}(\rho,\phi,z)$ on the side of the cylinder (see Fig. 3) is given by

$$\overline{g}(\rho,\phi,z)=\lim_{\delta\to 0}\delta^{1/3}\frac{1}{4\pi}\frac{\partial}{\delta\partial\phi'}\bigg|_{\phi'=0}g(\rho,\phi,z), \tag{12}$$

that is,

$$\overline{g}(\rho=a,\phi,z)=\frac{1}{\Gamma(5/3)2^{2/3}}\frac{2}{3\pi La}\sum_{n=1}^{\infty}\sin\left(\frac{2}{3}\phi\right)\times\sin\left(\frac{n\pi z}{L}\right)\sin\left(\frac{n\pi z'}{L}\right)\left(\frac{n\pi}{L}\right)^{2/3}\frac{1}{I_{2/3}\left(\frac{n\pi a}{L}\right)}. \tag{13}$$

On the end caps of the cylinder, this function is given by

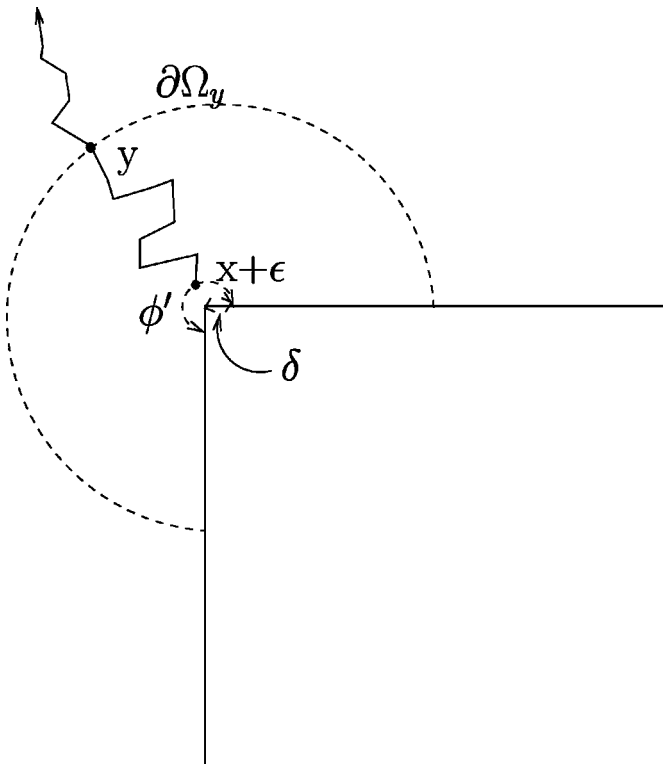

FIG. 3. Calculation procedure for the function $\overline{g}(x,y)$ that gives the (singular) probability density associated with a diffusing particle leaving the edge of an absorbing cube at the point x, and making first passage at the point y on the surrounding cylinder. Calculation requires two steps: first the angle ϕ' is taken to zero, putting the absorbing particle on the surface of the cube. Then the length δ is taken to zero, putting the diffusing particle on the edge.

$$\overline{g}(\rho,\phi,z=0)=\frac{1}{\Gamma(5/3)2^{2/3}}\frac{2}{3\pi L}\sum_{n=1}^{\infty}\sin\left(\frac{2}{3}\phi\right)\times\left(\frac{n\pi}{L}\right)^{5/3}\sin\left(\frac{n\pi z'}{L}\right)\frac{1}{I_{2/3}\left(\frac{n\pi a}{L}\right)}\times\left[I_{2/3}\left(\frac{n\pi a}{L}\right)K_{2/3}\left(\frac{n\pi\rho}{L}\right)-K_{2/3}\left(\frac{n\pi a}{L}\right)I_{2/3}\left(\frac{n\pi\rho}{L}\right)\right]. \tag{14}$$

For the edge distribution of a cube (see Fig. 2), $\sigma_e(x)$ is obtained as

$$\sigma_e(x)=2\int_0^a\int_0^{3\pi/2}\overline{g}(\rho,\phi)_{z=0}P(y)\rho\,d\rho\,d\phi+a\int_0^L\int_0^{3\pi/2}\overline{g}(\phi,z)_{\rho=a}P(y)d\phi\,dz. \tag{15}$$

IV. NUMERICAL RESULTS FOR EDGE DISTRIBUTIONS

In this section, we present our results for the charge singularities of the problem studied in this paper: a conducting

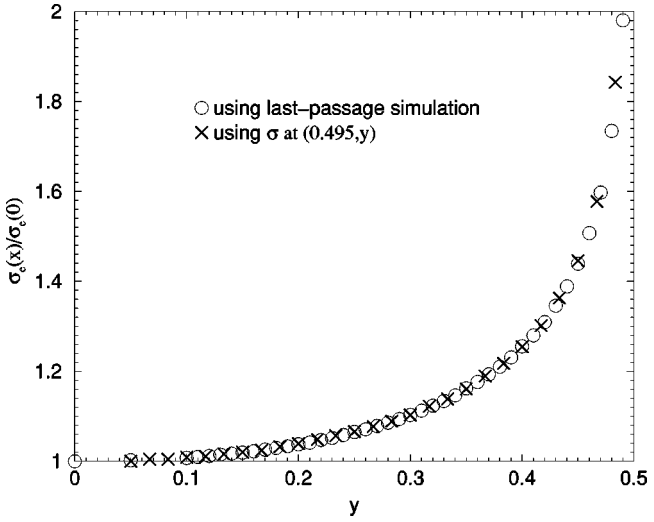

FIG. 4. The edge distribution of a unit cube calculated using Eq. (9) (crosses) and using Eq. (15) (circles). The edge distribution is shown rescaled with the value at the center of the edge of the cube. Here, y is the distance from the center of the edge of the cube.

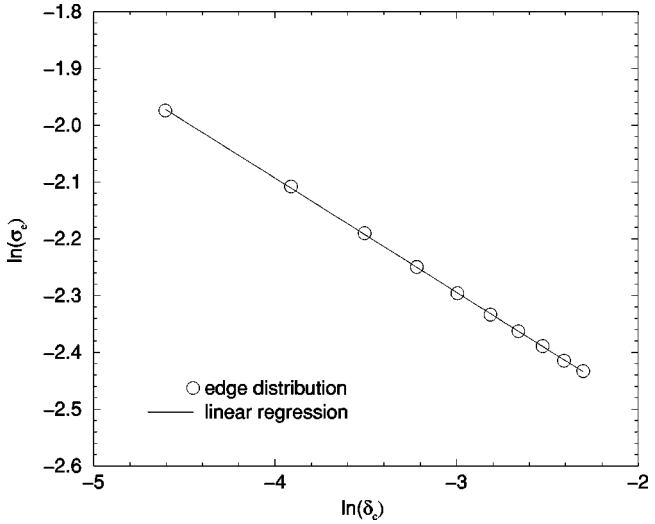

FIG. 5. Asymptotic edge distribution values near the corner of the edge distribution for a unit cube: δ_c is the distance along the edge from the corner and the linear regression slope is -0.2048, that is, $\sigma_e \sim \delta_c^{-0.2048}$.

cube. We will calculate the edge distribution of the conducting cube using two different methods.

We obtain the edge distribution of the absorbing cube in two ways: simulation using the last-passage method together with Eqs. (12)–(14) and direct simulation using Eq. (10). Both calculations utilize 10^8 Brownian motion paths. They both determine absorption using the WOS method, with an absorption layer of thickness 10^{-12}. This should produce accuracy of three to four decimal places. In calculating the edge distribution Green's functions for these two problems, a chopped cylinder of $L=a=0.002$ is used and the edge calculations are done at the center of the chopped cylinder on a cube moving the chopped cylinder along the edge of the cube (see Fig. 2). Due to the symmetry of both problems, the edge distribution is obtained in the range of 0–0.499 with 0.001 step. The result is shown in Fig. 4. The corner singularity of the cube is obtained using a least-squares fit as $\gamma \sim 0.2048 \pm 0.001$ in Fig. 5, where the best result using boundary element methods is 0.2134 [25]. It seems very difficult to obtain an accurate result for the corner singularity by attempting to extrapolate the edge distribution, at least for problems (such as the conducting cube) in which the corner singularity is relatively soft. It would be interesting to obtain a direct formula for the behavior near the corner by repeating the process used above to obtain the edge distribution. But this seems impossible: one knows the edge singularity, but not the corner singularity, exactly. So we do not obtain a last-passage algorithm for the corner singularity. In the following section we offer a first-passage algorithm for this quantity.

V. A FIRST-PASSAGE ALGORITHM FOR THE CORNER SINGULARITY

In this section, we present a diffusion-based simulation method that rapidly evaluates the power-law singularity associated with a corner of a conducting object. We also discuss its relation to the previous work.

Close enough to the corner singularity, the surface charge density on a charged conductor will be dominated by a single, power-law singularity of the form

$$\sigma(x) = A|x|^{\pi/\alpha - 1 - \gamma}. \tag{16}$$

This implies that the corresponding dominant term in the expansion of the voltage will be

$$\Phi(x) = A'|x|^{\pi/\alpha - \gamma}. \tag{17}$$

This can be proved in general by the discrete nature of the spectrum of the appropriate Laplacian eigenvalue problem. Here we assume that this dominance occurs at distances sufficiently far from the singularity so that one can do accurate Monte Carlo calculations of the voltage at such distances from the singularity. By the basic isomorphism of probabilistic potential theory, the voltage is equal to the fraction of diffusing particle that starts at a point external to the absorbing object and never contacts it. This is small near the corner singularity. Ideally, one would like to have a last-passage algorithm for this quantity. However, it seems to be inherently difficult to find one. Instead we use the Green's-function first-passage method [15] to obtain this quantity at distances $x_1 = 10^{-4}$ and $x_2 = 10^{-5}$ from the singularity. In terms of the corresponding voltages Φ_1 and Φ_2, we have from Eq. (2):

$$\frac{\pi}{\alpha} - \gamma = \ln\frac{\Phi_1}{\Phi_2} \Big/ \ln\frac{x_1}{x_2}. \tag{18}$$

Application of this method gives for the corner singularity of the conducting cube the result $\gamma = 0.2125$ and is in good agreement with the boundary element result presented in the last section.

We note that our results here are entirely consistent with those presented in the paper by Zhang and Zemanian [24]. Those authors present a formula for the total surface charge Q contained within a distance d of a corner of a conducting cube. This formula requires a calculation of the prefactor A' in Eq. (16) for the charge density. We do not provide this here. However, our method for determining corner singularities is completely general; it is not limited to the geometry of the cube.

VI. DISCUSSIONS AND CONCLUSIONS

This paper provides an important extension to last-passage Monte Carlo methods, allowing the treatment of problems containing boundary singularities. Important application areas include molecular biophysics and the materials science of composites.

An additional benefit of the edge distribution method is that it provides an efficient, flexible tool for the study of corner singularities, i.e., the power-law divergences that characterize the behavior of solutions to elliptic PDE's near corners.

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