A Monte Carlo Method for the Dirichlet Problem of Dielectric Wedges

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Abstract—**The Monte Carlo method considered here can be used to numerically compute electrostatic potentials inside a closed surface where a) the potential on the surface is known and b) the dielectric constant inside the surface changes only on boundaries. In this paper a modification is proposed to previously employed Monte Carlo methods, to overcome problems presented by dielectric wedges. In addition it is shown how it can be easily determined whether or not a point is inside a given domain. The connection between this topological problem and the Monte Carlo technique is explained.**

I. Introduction

CONSIDER the Dirichlet problem for the potential function V on a two-dimensional domain G:

$$\nabla\cdot(\epsilon\nabla V(x)) = 0 \qquad \text{for } x \in G$$
$$V(x) = V_0(x) \qquad \text{on the boundary } \partial G \quad (1)$$

where ϵ denotes the permittivity, which is constant in certain subdomains. Since it is not always possible to find an analytic solution for (1), many numerical methods have been developed. A special class of these methods form the Monte Carlo techniques which result from the so-called probabilistic potential theory.

It was shown by Kakutani [1] in 1944 that there is a mathematical relation between the Brownian motion of a particle and potential theory. Since then this theory has been extended and improved by many authors (e.g. [2]–[4]). For a comprehensive review of the subject the reader is referred to Griego and Hersh [5].

To get an idea of how the solution of problem (1) is computed by means of the Monte Carlo technique, imagine a particle undergoing Brownian motion inside a region G. The moving particle is released from point M and after some time will hit the boundary at a certain point $x \in \partial G$. Now repeat this moving-particle experiment n times. Then the potential in M is given by the expected value of the potentials at the boundary points $x_i \in \partial G$[6]:

$$V(M) = \lim_{n\to\infty} \sum_{i=1}^{n} V(x_i)/n. \quad (2)$$

In order to obtain a reasonable approximation of the potential the experiment (called the *random-walk process* in terms of Monte Carlo notation) has to be repeated many times. Of course we want the simulated random walk to be as efficient as possible. One might employ a grid of points (seperated by h) in domain G and random walk from point to point. The accuracy of the method would obviously depend on h: the smaller h the more accurate the computed potential. Halving the width of the grid means at least a fourfold increase in computing time (for a more precise analysis see also [7]). Muller [8] showed that the step size need not be small for all positions of the point and he proposed the *maximum-sphere procedure*. Royer [6] employed the maximum-sphere technique in his procedure. In spite of his efforts, some difficulties remained unsolved. In order to show this, we briefly describe Royer's technique below.

Let us define the *maximum sphere* [8] as the largest sphere $S(x_0)$ with center at x_0 which is entirely contained in G; obviously the radius of this sphere is given by

$$r = \inf_{x\in\partial G} |x - x_0|. \quad (3)$$

The maximum-sphere process is the procedure of computing the maximum sphere of a given point, generating a uniformly and randomly distributed position on the surface of the sphere, and continuing this process iteratively at the new position until the process hits the boundary.

In technical applications of (1), e.g. in transmission line problems, the domain G frequently is seperated into subdomains of different dielectrical properties ϵ_i. The potential has to fulfill certain continuity and jump relations at the interfaces ∂I of these subdomains. It will be seen that it is useful to modify the definition of the maximum sphere $S(x_0)$ with radius

$$r_I = \inf_{x\in\partial I,\,\partial G} |x - x_0| \quad (4)$$

whereby x_0 denotes again the center of the sphere. In words, this means that a small sphere with center at x_0 would be expanded as much as any boundary ∂I or ∂G would allow (Fig. 1).

Step by step, the procedure is as follows:

1) The process starts in $x_0 := M$, where we wish to compute the potential $V(M)$.
2) Determine the maximum sphere $S(x_i)$ at x_i with the help of (4).
3) The point x_{i+1} is selected uniformly and randomly on $S(x_i)$.

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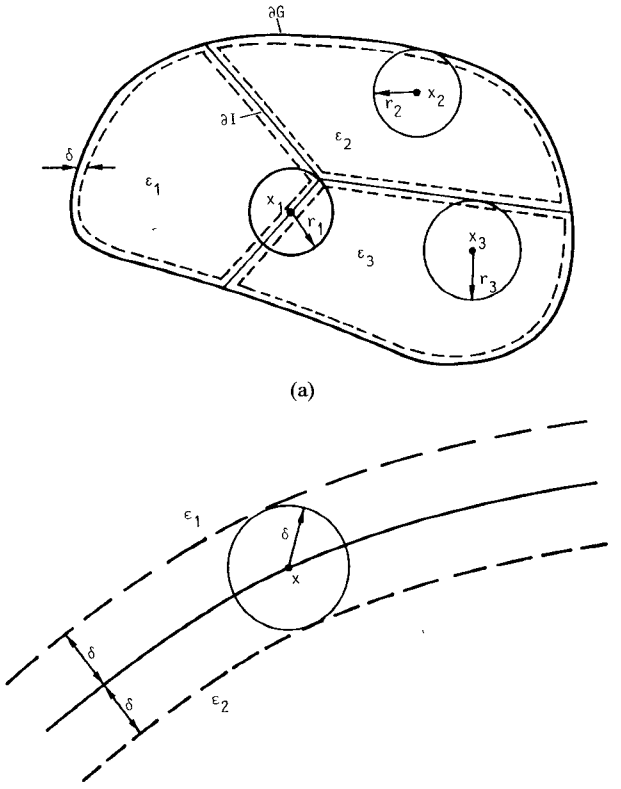

Fig. 1. Choice of the (maximum) sphere in different situations of the maximum-sphere process. (a) x_1 is nearest to a dielectric edge, x_2 to ∂G, and x_3 to ∂I. (b) If x is found on a curved dielectric interface, the radius of the sphere is $r_s = \delta$ to ensure that the curved interface is approximately a straight line within the sphere.

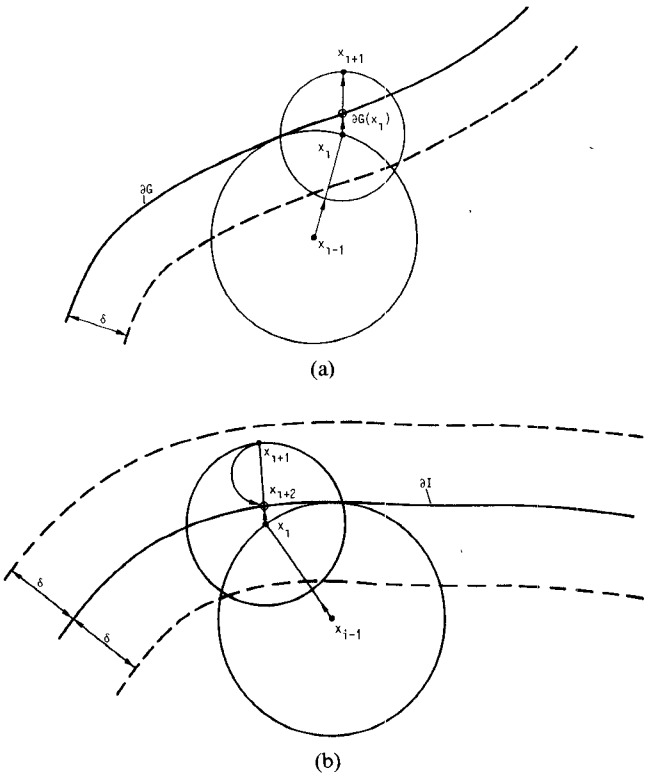

Fig. 2. The spherical process enters the δ neighborhood of (a) the boundary ∂G: $V(\partial G(x_i))$ is the resulting potential of the experiment; (b) the boundary ∂I: x_{i+2} is the position of relocation when crossing the boundary.

Note that, as has been shown in [8], that the maximum-sphere process converges to the boundary ∂G of the domain G with probability 1. In practice, the process must be interrupted at some small maximum-sphere radius r_I to avoid computation times which are too long. Accordingly, each ∂I and ∂G has adjoining regions which are δ wide (see Fig. 1). For more details and an error estimation see [6]. Continuing our description of the procedure, incorporating dielectric boundaries, we have:

4) In case a position x_i generated randomly is entering a δ neighborhood of (cf. Fig. 2)
   a) the boundary ∂G: Generate a position x_{i+1} uniformly and randomly on a sphere with radius δ. If the new position has crossed the boundary ∂G the random walk is terminated and the potential at $\partial G(x_i)$ is noted for use in (2). Otherwise continue the process as above.
   b) the boundary ∂I: Generate a position x_{i+1} uniformly and randomly on a sphere with radius δ. If the new position has not crossed the interface continue as defined above. Otherwise relocate the process on the point of intersection x_{i+2} of the interface and the straight line between x_i and x_{i+1}. Now choose a sphere with center x_{i+2} and radius r_S which is small compared to the radius of curvature of the dielectric boundary (Fig. 1(b)).

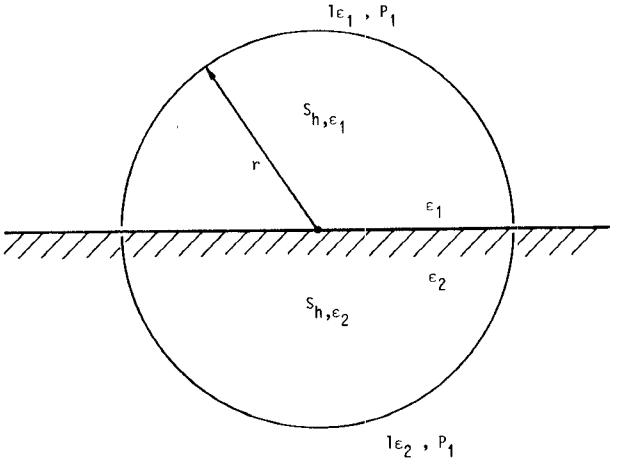

Fig. 3. Configuration to describe the use of the transition probabilities determined by (5) and (6).

This guarantees that the dielectric boundary enclosed by the sphere appears like a straight line (in two dimensions). If the interface is not curved select the maximum sphere. To take the change in permittivity within the sphere into account, jump into the region designated by ϵ_1 with probability (Fig. 3)

$$p_1 = \epsilon_1/(\epsilon_1 + \epsilon_2) \tag{5}$$

and into the dielectric ϵ_2 with probability

$$p_2 = 1 - p_1 = \epsilon_2/(\epsilon_1 + \epsilon_2). \tag{6}$$

Now select a new position x_{i+3} uniformly at random either on the half-sphere $S_{h,\epsilon_1}(x_{i+2})$ or $S_{h,\epsilon_2}(x_{i+2})$ according to (5) and (6). Continue the process as defined above.

The probabilities p_1 and p_2 are called *transition probabilities* for the associated dielectrics ϵ_1 and ϵ_2. The calculation of these has been carried out by Royer [6]. For the case where the point x_{i+2}, mentioned in b) of step 4), is the vertex of a dielectric wedge (or, better, is very close to a dielectric edge since the probability of catching a point in a continuous distribution is zero), a difficulty occurs. Inasmuch as the radius of curvature of a vertex is zero, the above-mentioned sphere must have a radius going to or equal to zero. This would cause a degeneration of the process.

It is the purpose of this paper to present some ideas to overcome this dilemma. We determine the transition probabilities for a position of the process located on or near the vertex of dielectric wedges and show how to choose the sphere in this situation.

II. Transition Probabilities

Consider n dielectric plane wedges of permittivity ϵ_i and opening angles θ_i with vertices unified in M (Fig. 4). Given the potential $V(a,\varphi)$ on a cylinder $r=a$ as a function of φ, we want to compute the potential $V(M)$ in M. We begin with Gauss's theorem [9] in homogeneous charge-free space:

$$\iint_S D_n dS = 0 \tag{7}$$

where D_n denotes the normal component of the electric displacement and dS the surface element of the closed surface S.

Considering only cylindrical problems, Gauss's theorem can be reduced to

$$\oint_l D_n dl = 0 \tag{8}$$

where dl denotes the curve element.

The electric displacement in the radial direction $\vec{e}_r$ can be written as

$$D_n = \epsilon E_r(r,\varphi). \tag{9}$$

Expressing the curve element in terms of the angle φ,

$$dl = r\,d\varphi \tag{10}$$

Gauss's theorem becomes

$$\int_l \epsilon E_r(r,\varphi) r\,d\varphi = 0. \tag{11}$$

Since the cylinder in $r=a$ encloses regions with different dielectrics, we have to integrate piecewise over the circular arcs $l_i = l_i(r)(i=1,\cdots,n)$ weighted by ϵ_i:

$$\sum_{i=1}^{n} \int_{l_i} \epsilon_i E_{ir}(r,\varphi) r\,d\varphi = 0. \tag{12}$$

Since the integration in (12) is with respect to φ, we may

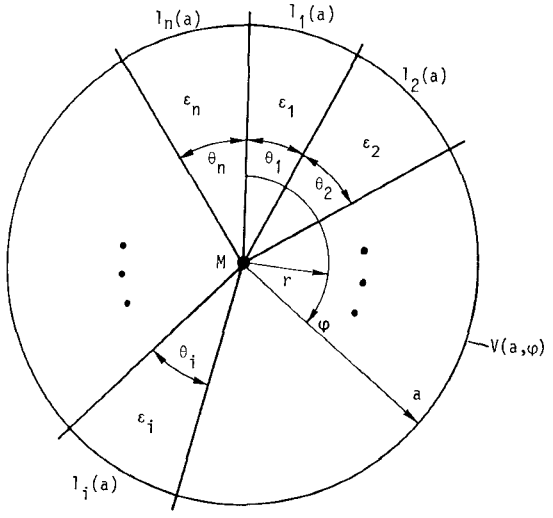

Fig. 4. Dielectric wedges with center in M, given the potential $V(a,\varphi)$.

factor r and then integrate with respect to r:

$$\sum_{i=1}^{n} \int_0^a \int_{l_i} \epsilon_i E_{ir}(r,\varphi)\,d\varphi\,dr = 0. \tag{13}$$

Changing the order of integration:

$$\sum_{i=1}^{n} \int_{l_i} \int_0^a \epsilon_i E_{ir}(r,\varphi)\,dr\,d\varphi = 0 \tag{14}$$

and representing the integral over r by the potentials of the limits:

$$\int_0^a E(r)\,dr = V(0) - V(a) \tag{15}$$

(14) becomes

$$\sum_{i=1}^{n} \int_{l_i} \epsilon_i [V_i(0,\varphi) - V_i(a,\varphi)]\,d\varphi = 0. \tag{16}$$

Furthermore, since $V_i(0,\varphi)$ is the desired potential $V(M)$:

$$V_i(0,\varphi) = V(M), \qquad i=1,\cdots,n \tag{17}$$

(16) results in

$$\sum_{i=1}^{n} \int_{l_i} \epsilon_i V(M)\,d\varphi = \sum_{i=1}^{n} \int_{l_i} \epsilon_i V_i(a,\varphi)\,d\varphi. \tag{18}$$

The integrand on the left-hand side of (18) does not depend on φ and therefore (18) simplifies to

$$V(M) \cdot \sum_{i=1}^{n} \epsilon_i \theta_i = \sum_{i=1}^{n} \int_{l_i} \epsilon_i V_i(a,\varphi)\,d\varphi \tag{19}$$

which leads to the result

$$V(M) = \sum_{i=1}^{n} \frac{\epsilon_i \theta_i}{\sum_{j=1}^{n} \epsilon_j \theta_j} \left[\frac{1}{\theta_i a} \int_{l_i} V_i(a,\varphi)\,dl \right] \tag{20}$$

by resetting $dl = a\,d\varphi$. We explain the factor

$$p_i = \frac{\epsilon_i \theta_i}{\sum_{j=1}^{n} \epsilon_j \theta_j} \tag{21}$$

as the transition probabilities searched for. Since $p_i \geq 0$ and the conservation relation $\sum_{i=1}^{n} p_i = 1$ holds, it is ensured that the p_i are in fact probabilities.

Note that the radius a in (20) has been chosen arbitrarily. This implies a feasible expansion of the sphere $S(M)$ to the maximum sphere defined by (4). Now we are able to complete the description of the maximum-sphere process begun in the Introduction, adding:

4) c) a dielectric edge (vertex): Displace x_i exactly[1] to the dielectric edge x_{i+1}. Determine the maximum sphere $S(x_{i+1})$, which encloses now n wedges with dielectric ϵ_k. Generate a position x_{i+2} uniformly and randomly on the circular arc l_k determined at random with the help of (21).

As a special case we consider the straight line ($n = 2$, $\theta_1 = \theta_2 = \pi$). Simplification of (20) yields:

$$V(M) = \frac{\epsilon_1}{\epsilon_1 + \epsilon_2}\left[\frac{1}{\pi a}\int_{l_1} V\,dl\right] + \frac{\epsilon_2}{\epsilon_1 + \epsilon_2}\left[\frac{1}{\pi a}\int_{l_2} V\,dl\right]. \quad (22)$$

The solution thus reduces to that presented in [6, eq. (12)].

III. A Topological Method

For the purpose of a simple computation of the maximum sphere and the determination whether a boundary has been crossed, it is necessary to compute the domain G in which the randomly walking point is located. The method which we will use to make the above computation employs the following theorem.

Theorem: Suppose D is a convex domain with smooth boundary ∂D in the Euclidean plane $\mathbb{R}^2$ and $\vec{z}_0 \notin \partial D$. Let $\vec{P}z_0 \in \partial D$ be defined as the orthogonal projection of $\vec{z}_0$ onto ∂D; i.e., we have

$$r = \inf_{\vec{z} \in \partial D} |\vec{z} - \vec{z}_0| = |\vec{P}z_0 - \vec{z}_0|. \quad (23)$$

If $\vec{n}$ denotes the outer normal with respect to D at $\vec{P}z_0$, then the following are equivalent:

$$\text{(i)} \quad \vec{n} = \frac{\vec{P}z_0 - \vec{z}_0}{|\vec{P}z_0 - \vec{z}_0|} \quad (24)$$

$$\text{(ii)} \quad \vec{z}_0 \in D.$$

For illustration see Fig. 5(a).

Remarks: In this theorem we assumed for simplicity that D is convex (this determines the orthogonal projection $\vec{P}z_0$ uniquely) and that ∂D is smooth (this ensures the existence of a unique outer normal at each point $\vec{z} \in \partial D$). Below we show how to deal with a general simply connected domain bounded by a polygonal curve. For such domains it is very easy to compute the outer normals explicitly and so the theorem can be used quite effectively. In a polygonal curve proceed as follows: Extend the polygon sides connected with this edge beyond the edge point,

[1] This displacement avoids degeneration of the process. We have to allow the small error which takes place by this procedure. The method of testing for an intersection close to an edge by analogy with 4) a) and b) does not make sense since the dimension of the edge point is zero.

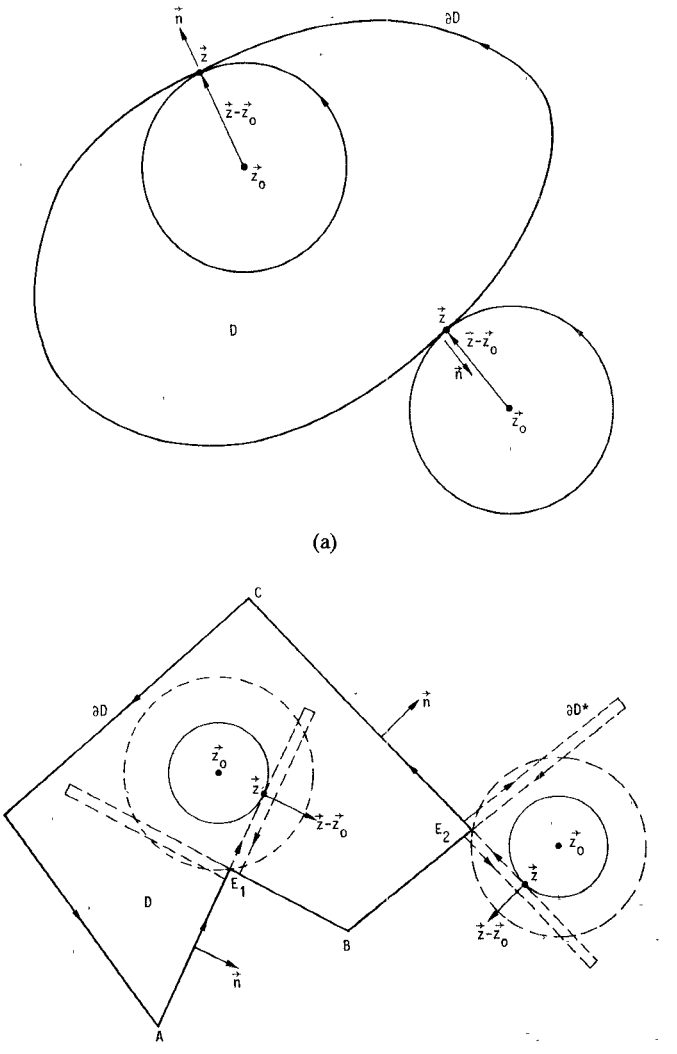

Fig. 5. How to decide whether a given position $\vec{z}_0$ is inside or outside a predefined domain D. (a) If the outer normal in $\vec{z}$ has the same direction as $\vec{z} - \vec{z}_0$ it follows that $\vec{z}_0 \in D$. (b) In the case where ∂D is a polygon it is possible that $\vec{z}_0$ is near an edge point E. In this situation the extensions of $\overline{AE_1}$, $\overline{BE_1}$ and $\overline{CE_2}$, $\overline{BE_2}$ give information about the site of $\vec{z}_0$ in relation to D.

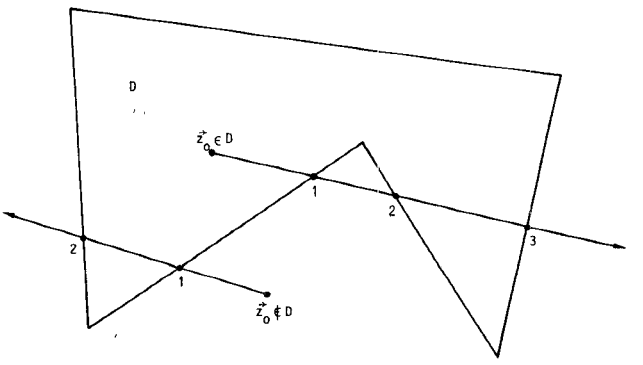

Fig. 6. The procedure of Meschkowski [12] to determine the site of a point $\vec{z}_0$ in relation to a given domain D. If the number of intersections is odd, $\vec{z}_0 \in D$; otherwise $\vec{z}_0 \notin D$.

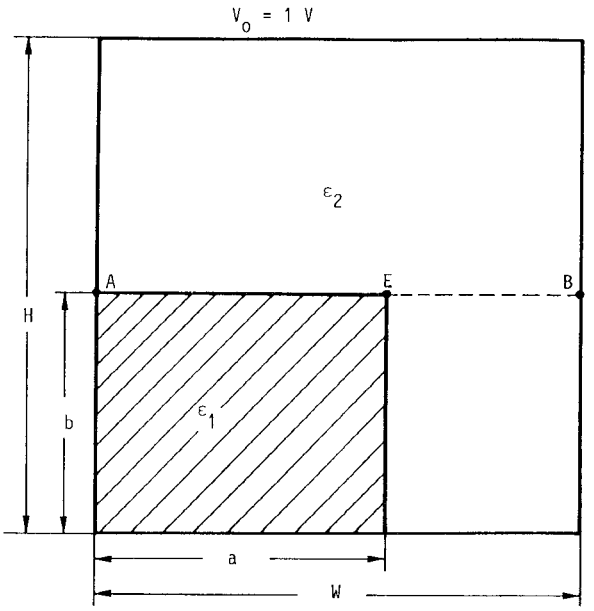

Fig. 7. The box used for the sample calculations. The potentials of the right, left and lower sides are zero. The upper side has the potential 1 V.

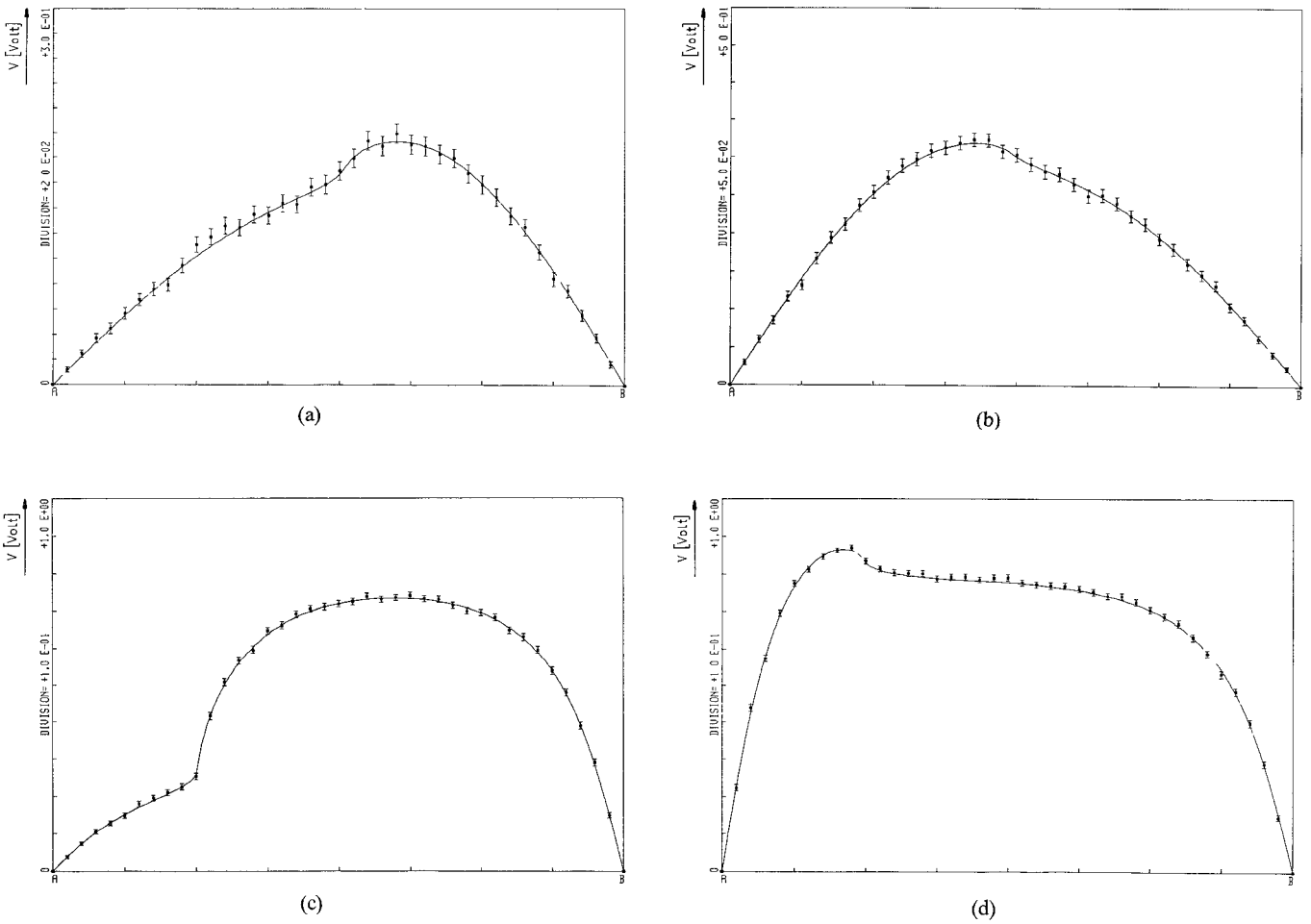

Fig. 8. Sample calculations for the configuration shown in Fig. 7. The common parameters are $\delta/H = 0.0005$; 95 percent confidence limits and the number of random walks was 10 000. (a) $a/W = 0.5$; $b/H = 0.5$; $W/H = 1.0$; $\epsilon_1/\epsilon_0 = 3$; $\epsilon_2/\epsilon_0 = 1$. (b) $a/W = 0.5$; $b/H = 0.5$; $W/H = 1.0$; $\epsilon_1/\epsilon_0 = 1$; $\epsilon_2/\epsilon_0 = 3$. (c) $a/W = 0.25$; $b/H = 0.8$; $W/H = 2.0$; $\epsilon_1/\epsilon_0 = 10$; $\epsilon_2/\epsilon_0 = 1$. (d) $a/W = 0.25$; $b/H = 0.8$; $W/H = 2.0$; $\epsilon_1/\epsilon_0 = 1$; $\epsilon_2/\epsilon_0 = 10$.

which now becomes the intersection of two straight lines (see Fig. 5(b)). Using the new polygon ∂D^* and the above theorem decide whether or not $\vec{z}_0 \in D$.

Note that the extrapolations of the above-mentioned polygon sides have the same outer normal as the polygon sides themselves. This modification of the polygon ∂D does not change the topology as long as $\vec{z}_0$ remains in $\partial D^*(\vec{z}_0 \in \partial D^*$ and $\vec{z}_0 \notin \partial D$ is the limiting case in which the outer normal of $\vec{z} \in \partial D$ just exists).

The proof can be outlined as follows [10]: Consider the maximum sphere $S(\vec{z}_0)$ with positive orientation of its boundary ∂S. Assume the same orientation for the boundary ∂D. The winding number $n(\Gamma, z_0)$ (here we make use of the isomorphism $\mathbb{R}^2 \cong \mathbb{C}$) of a point z_0 in the complex plane $\mathbb{C}$ with respect to a simple closed curve Γ [11] determines whether z_0 is inside or outside of Γ depending on whether $n(\Gamma, z_0) = 1$ or 0. The homotopy property [11] of the winding number and knowledge of the outer normals at a sphere shows that $\vec{n}$ has the same direction as $\vec{z} - \vec{z}_0$ if and only if $\vec{z}_0 \in D$.

We have not been able to find the above theorem anywhere in the literature. Meschkowski [12], however, describes another technique for determining whether or not $\vec{z}_0 \in D$. The procedure involves counting the number of intersections of a ray, originating at $\vec{z}_0$, makes with the boundary ∂D. If this number is odd, $\vec{z}_0 \in D$; otherwise $\vec{z}_0 \notin D$ (for illustration see Fig. 6).

The advantage of our procedure stems from the conformity of (23) and (4). Equation (23) describes nothing less than the maximum sphere in a general domain (which may be G or a subdomain boundary by ∂G or ∂I). The benefit in programming expense is obvious since the procedure for computing the maximum sphere must be carried out anyway.

IV. An Example

Consider a rectangular dielectric wedge ($n = 2$, $\theta_1 = \pi/2$, $\theta_2 = 3\pi/2$). In this case, (21) yields the transition probabilities

$$p_1 = \epsilon_1/(\epsilon_1 + 3\epsilon_2) \qquad \text{for the circular arc } l_1 \quad (25)$$

and

$$p_2 = 3\epsilon_2/(\epsilon_1 + 3\epsilon_2) \qquad \text{for the circular arc } l_2. \quad (26)$$

The dielectric wedge is embedded into a potential box (Fig. 7) whose sides are at potential 0 with the exception of the upper side, which is at potential $V_0 = 1$ V. We have computed the potential on the straight line $\overline{AB}$. The dielectrics ϵ_1 and ϵ_2 are viewed as parameters (see Fig. 8(a)–(d)). The confidence limits are calculated with the method derived by Royer [6]. The number of random walks executed was $N = 10\,000$. The curves plotted in Fig. 8(a)–(d) are the exact solutions obtained by application of the finite difference method and an overrelaxation algorithm [13]. The representation of the dielectric edge as well as the interface in terms of finite differences has been established by Green [14].

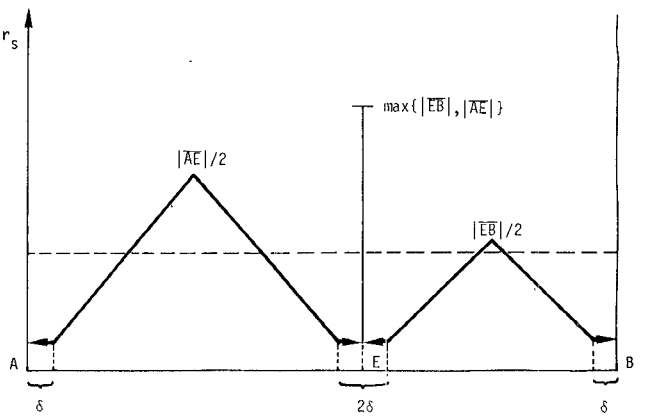

Fig. 9. The radius r_s of the maximum sphere for points on the straight line $\overline{AB}$. A small range of relocation δ is to take into account to avoid a degeneration of the maximum-sphere process.

A comparative study of the Monte Carlo method and finite element method was presented in [15]. However, in that paper the Monte Carlo method was not implemented for dielectric boundaries.

Since in our example the process was always started from the straight line $\overline{AB}$, it is interesting to consider the radius of the maximum sphere r_s for points on the straight line $\overline{AB}$ (Fig. 9). The method developed in this paper makes it possible to choose the maximum sphere with radius $r_s = \max\{|\overline{EB}|, |\overline{EA}|\}$ when the process is entering the δ neighborhood of E. The conditions in Fig. 9 have been chosen such that the maximum sphere is not affected by the top and bottom of the box. Otherwise the vertices of the function in Fig. 9 are cut off as indicated by the broken line.

V. Conclusions

In accordance with Royer [6] one could say that "the method may... be useful for spot-checking potentials obtained by other methods or for solving problems for which only a few potentials are required."

Since the recent appearence of vector machines, the importance of the Monte Carlo method is growing. Utilizing the special architecture of these computers, it is possible to process several random walks in parallel, which reduces computation time considerably.

Carrying out calculations at high speed and with sufficient accuracy for domains with arbitrary curved boundaries is still quite difficult. Nevertheless, the Monte Carlo technique and the further development in this paper allow computation of the potentials for domains with different dielectrics bounded by arbitrary polygon curves.

With the aid of the theorem stated in Section III, it is possible to detect whether a given point $\vec{z}_0$ is inside or outside a domain D. Although the theorem is valid for any boundary curve ∂D, the application is recommended only if the outer normal of each point $\vec{z} \in \partial D$ is known before computation starts. This requirement is easy to perform if the boundary curve ∂D is represented by a polygon, which

has only a finite number of outer normals at the boundary ∂G.

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