Monte Carlo diffusion algorithms are a powerful, versatile method of solving elliptic, partial differential equations. With the aid of probabilistic potential theory [1], many practical problems can be framed in terms of generalized diffusion equations, whose solutions are expressed as averages over the trajectories of diffusing particles. Because each particle executes Brownian motion independently of the others, such problems are naturally adapted to parallel computation. Because diffusing particles interact only locally with their environment, problems involving irregular and convoluted boundaries are readily treated [2].

In particular, diffusion Monte Carlo algorithms [3–5] map electrostatic problems onto diffusion problems: charges become point sources of diffusing particles, and conductors become perfect absorbers of these particles.

Two major growth areas, biotechnology [3,6] and micro-fabrication [7,8], are domains making heavy use of these methods. Here we focus on the latter. The ever-decreasing length scales involved in semiconductor device fabrication have made the three-dimensional (3D) interconnect geometry more complex and interconnect capacitance important because the parasitic capacitance is a dominant factor in high-speed chip design [7]. A Monte Carlo method, the floating random-walk method, has been used for extracting the capacitance of complex 3D interconnects for integrated circuits [8]. This method is a detailed application of the Feynman-Kac theorem; it allows calculation of the potential (and the surface charge density) at a point as a weighted average over the boundary values.

First-passage Monte Carlo diffusion algorithms are known to be quite efficient and accurate for calculating the simple capacitance of a conductor [2,3]. The conductor becomes an absorbing object of identical size and shape. The capacitance is related to the fraction of diffusing particles that start at random positions on a sphere surrounding this absorbing object, and are absorbed at its surface. These methods are efficient, because they are charge based, i.e., they focus on computing the surface charge distribution. On the one hand, the entire potential distribution can be obtained from the surface charge distribution, e.g., by the fast multipole method [9]. On the other hand, first-passage methods automatically incorporate importance sampling; thus, they are computationally fast. But first-passage methods seem not to generalize to the problem of mutual capacitance.

In this paper, we introduce a last-passage diffusion algorithm [9,10], a Monte Carlo method, which does allow calculation of mutual capacitance. In this method, we average over diffusion paths that start very near to one of the absorbing objects and diffuse until they are either absorbed by a different absorbing object, or diffuse away to infinity.

The mutual capacitance matrix $C_{ji}$ of a set of $N$ conductors is defined by the relation

$$Q_j = \sum_{i=1}^{N} C_{ji} V_i.$$  \hfill (1)

Here, $V_j$ and $Q_j$ are, respectively, the voltage and charge on the $j$th conductor. $C_{ji}$ is the total charge on conductor $j$, when one applies unit voltage to conductor $i$ while grounding all the other conductors. It is the integral, over the surface of conductor, $j$, of surface charge $\sigma_j$. The voltage field $V(x)$ thus imposed is identical to the function $P(x \to C)$, which is the probability that a diffusing particle started at the point $x$ will be absorbed on the surface $C'$ of the $i$th conductor. By Gauss’s law, the surface charge density $\sigma_j(x)$ is given by

$$\sigma_j(x) = \frac{d}{d\epsilon} \left|_{\epsilon=0} \right. \lim_{\epsilon \to 0} \frac{P[(x+\epsilon) \to C'] - 1}{\epsilon}.$$  \hfill (2)

Except for a minus sign, the numerator of this expression is the probability that a diffusing particle starting at $(x+\epsilon)$ will not be absorbed on the $i$th surface. The $\epsilon \to 0$ limit is evaluated as follows: The probability $P[(x+\epsilon) \to C']$ can be written as a convolution of two factors: the probability $g(x + \epsilon, y)$ that a diffusing particle leaves point $(x+\epsilon)$ and makes first passage at a point $y$ on a sphere of radius $a$ surrounding point $x$; and the probability $[1 - P(y \to C')]$ that a particle started at the point $y$ is absorbed by a conductor other than the $i$th, or wanders off to infinity. The first factor is proportional to $\epsilon$, but is simple. The second factor can be obtained via Monte Carlo simulation. Thus $C_{ji}$ is given by

Last-passage Monte Carlo algorithm for mutual capacitance

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We develop and test the last-passage diffusion algorithm, a charge-based Monte Carlo algorithm, for the mutual capacitance of a system of conductors. The first-passage algorithm is highly efficient because it is charge based and incorporates importance sampling; it averages over the properties of Brownian paths that initiate outside the conductor and terminate on its surface. However, this algorithm does not seem to generalize to mutual capacitance problems. The last-passage algorithm, in a sense, is the time reversal of the first-passage algorithm; it involves averages over particles that initiate on an absorbing surface, leave that surface, and diffuse away to infinity. To validate this algorithm, we calculate the mutual capacitance matrix of the circular-disk parallel-plate capacitor and compare with the known numerical results. Good agreement is obtained.

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The capacitance matrix element $C_{ij}$ involves classes II and III; element $C_{12}$ involves class II. The function $G(x,y)$ is a propagator that moves diffusing particles from a point $x$ on the lower absorbing surface to a point $y$ on a surrounding sphere. [See Eqs. (3) and (7)].

$$C_{ij} = \oint_{x \in C^i} dS \sigma_i(x),$$  \hspace{1cm} (3)

$$\sigma_i(x) = \frac{1}{4\pi} \int d^2 y \; G(x,y)[1 - P(y \rightarrow C^i)].$$  \hspace{1cm} (4)

Here, $G(x,y)$ is the Laplacian Green’s function for a point dipole centered at point $x$ and normal to the surface,

$$G(x,y) = \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \; g(x + \epsilon y)$$  \hspace{1cm} (5)

where $g(x + \epsilon y)$ is the Laplacian Green’s function associated with Dirichlet boundary conditions on the region $\partial \Omega$. For a flat conducting surface, this dipole Green’s function is given by [11]

$$G(x,y) = \frac{3}{2\pi} \frac{\cos \theta}{a^3},$$  \hspace{1cm} (6)

where $\theta$ is the angle between the vectors $x$ and $y$.

The same ideas give for $C_{ij}, j \neq i$,

$$C_{ij} = \oint_{x \in C^i} dS \sigma_i(x),$$  \hspace{1cm} (7)

$$\sigma_i(x) = -\frac{1}{4\pi} \int d^2 y \; G(x,y)P(y \rightarrow C^i).$$  \hspace{1cm} (8)

The last-passage method is tested by calculating the mutual capacitance of the parallel-circular-plate capacitor [12]. The integrals over surface charge in Eqs. (3) and (7) are calculated using the fractional sampling method [13], with the reference for importance sampling of the charge distribution being the single charged circular plate. The fractional sampling method has been used extensively in neutron transport and similar problems.

The integrals over surface charge in Eqs. (3) and (7) are calculated using adaptive numerical integration [14] with the function evaluations of $\sigma_i$, $\sigma_j$ being defined by Eqs. (4) and (8). Each function evaluation is performed by choosing 100 points at random on the $y$ sphere surrounding point $x$, launching one diffusing particle from each point, and evaluating the function $P$ as either zero or unity depending on the outcome (see Fig. 1).

For each relative separation, $10^8$ diffusing particles were used. The absorption layer thickness for “walks on spheres” [5,15] was $10^{-6}$. In the region outside the plates we use “walks on planes” [16–18], a natural generalization.

The rather simple problem of a parallel-disk capacitor was studied here because a quasianalytic solution for this problem is available [12]; this gives us a reliable standard by which to evaluate our method. Carlson and Illman performed a numerical integration of Love’s equation, an integral equation of Fredholm type obeyed by the charge density in this problem. Specifically, they solved for the quantity $(C_{11} - C_{12})$, which is given by

$$(C_{11} - C_{12}) = 4\epsilon_0 a \int_0^1 f(r) dr$$  \hspace{1cm} (9)

where the charge density $f(r)$ obeys the equation

<table>
<thead>
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<th>$\ell$</th>
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<th>$C_{11} + C_{12}$ Analytic</th>
<th>$(C_{11} - C_{12})$ Monte Carlo</th>
<th>$(C_{11} + C_{12})$ Monte Carlo</th>
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</table>

The integral equation solved in that work.

FIG. 1. (Color online) Side view of particles diffusing in the geometry of a parallel-plate capacitor. Examples are shown of three classes of diffusing particle paths: (I) those that eventually diffuse back to the lower surface and are absorbed; (II) those that are absorbed on the upper surface; (III) those that diffuse away to infinity.
\[ f(r) = 1 + \int_0^1 K(r, s, \ell) f(s) ds \] (10)

with

\[ K(r, s, \ell) = \frac{\ell}{\pi} \left( \frac{1}{\ell^2 + (r + s)^2} + \frac{1}{\ell^2 + (r - s)^2} \right) \] (11)

and \( \ell = d/a \), the dimensionless plate separation. It can be easily seen that the quantity \( C_{11} + C_{12} \) is given by the same equation, but with the plus sign on the right-hand side of Eq. (10) replaced by a minus sign. We solved for this quantity following the approach of Carlson and Illman. Both sets of analytic results agree well with our Monte Carlo results (see Table I).

The last-passage algorithms can be made more efficient by incorporating importance sampling into the Monte Carlo process [19]. This is presently under study.

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