

Last-passage Monte Carlo algorithm for mutual capacitance

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(Received 7 February 2006; published 4 August 2006)

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.

DOI: [10.1103/PhysRevE.74.027701](https://doi.org/10.1103/PhysRevE.74.027701)

PACS number(s): 46.15.-x, 41.20.Cv, 05.40.Jc

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

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

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 σ_{ji} . The voltage field $V(x)$ thus imposed is identical to the function $P(x \rightarrow C^i)$, which is the probability that a diffusing particle started at the point x will be absorbed on the surface C^i of the i th conductor. By Gauss's law, the surface charge density $\sigma_{ii}(x)$ is given by

$$\sigma_{ii}(x) = \frac{d}{d\epsilon} \bigg|_{\epsilon=0} P[(x+\epsilon) \rightarrow C^i] = \lim_{\epsilon \rightarrow 0} \frac{P[(x+\epsilon) \rightarrow C^i] - 1}{\epsilon}. \quad (2)$$

Except for a minus sign, the numerator of this expression is the probability that a diffusing particle starting at $(\mathbf{x}+\epsilon)$ will not be absorbed on the i th surface. The $\epsilon \rightarrow 0$ limit is evaluated as follows: The probability $P[(x+\epsilon) \rightarrow C^i]$ 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 $[1 - P(y \rightarrow C^i)]$ 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 ϵ , but is simple. The second factor can be obtained via Monte Carlo simulation. Thus C_{ii} is given by

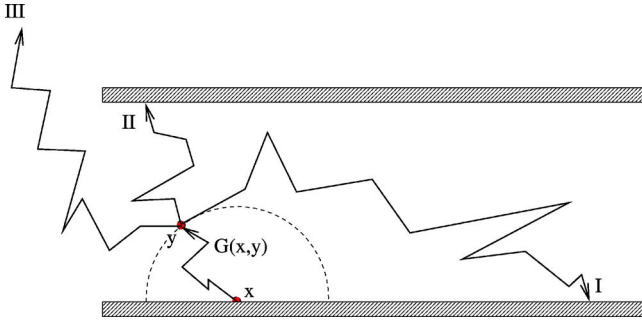


FIG. 1. (Color online) Side view of particles diffusing in the geometry of a parallel-plate capacitor. Examples are shown of three classes of diffusing particle paths: (I) those that eventually diffuse back to the lower surface and are absorbed; (II) those that are absorbed on the upper surface; (III) those that diffuse away to infinity. The capacitance matrix element C_{11} 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)].

$$C_{ii} = \oint_{x \in C^i} dS \sigma_{ii}(x), \quad (3)$$

$$\sigma_{ii}(x) = \frac{1}{4\pi} \oint d^2y G(x,y) [1 - P(y \rightarrow C^i)]. \quad (4)$$

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

$$G(\mathbf{x}, \mathbf{y}) = \left. \frac{d}{d\epsilon} g(\mathbf{x} + \epsilon, \mathbf{y}) \right|_{\epsilon=0} \quad (5)$$

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

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

where θ is the angle between the vectors x and y .

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

$$C_{ij} = \oint_{x \in C^i} dS \sigma_{ij}(x), \quad (7)$$

$$\sigma_{ij}(x) = -\frac{1}{4\pi} \oint d^2y G(x,y) P(y \rightarrow C^j). \quad (8)$$

The last-passage method is tested by calculating the mutual capacitance of the circular-disk parallel-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 σ_{ii} , σ_{ij} 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

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

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

TABLE I. Dimensionless capacitance coefficients $(\pi/a)C$ for the parallel-circular-plate capacitor. Analytic results are compared to Monte Carlo results for both independent mutual capacitance quantities in this problem, $(C_{11} - C_{12})$ and $(C_{11} + C_{12})$, as functions of $\ell = d/a$, the dimensionless plate separation. Here a is the radius of the circular plates and d their separation. Analytic results for the quantity $(C_{11} - C_{12})$ were taken from Ref. [12]; analytic results for $(C_{11} + C_{12})$ were calculated by the authors by solving a modification of the integral equation solved in that work.

ℓ	$(C_{11} - C_{12})$		$(C_{11} + C_{12})$	
	Analytic	Monte Carlo	Analytic	Monte Carlo
0.001	787.0	788.0	0.50070	0.5002
0.01	80.43	80.41	0.50537	0.50484
0.1	9.2331	9.2320	0.53588	0.53559
1	1.8208	1.8203	0.69120	0.69104
10	1.0675	1.0643	0.94051	0.94094

$$f(r) = 1 + \int_0^1 K(r,s, \ell) f(s) ds \quad (10)$$

with

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

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.

ACKNOWLEDGMENTS

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (Grant No. KRF-2005-005-J01103). Also, this work was supported partly by the Korean Ministry of Information & Communication through the Information Technology Research Center Program and Information Technology Professor Support Program supervised by the Institute of Information Technology Assessment (IITA), and partly by the Korean Ministry of Science and Technology (MOST) through the Korea Institute of Science and Technology Evaluation and Planning (KI-STEP).

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