An Improved Floating-Random-Walk Algorithm for Solving the Multi-Dielectric Dirichlet Problem

Jayant N. Jere and Yannick L. Le Coz

Abstract— **An improved floating-random-walk algorithm for solving the multi-dielectric Dirichlet problem is outlined. The improvement is achieved by using statistically generated Green's functions that are calculated before hand and stored as look-up tables. These tables have been used to solve the multi-dielectric Dirichlet problem for an arbitrary two dimensional geometry. The improved algorithm is also compared with the conventional floating-random-walk algorithm and is found to be at least two times more efficient. Results are presented for two types of parallel plate geometries.**

I. Introduction

RECENT interest has focused on the effect of high density interconnects in complex integrated circuits. Advances in lithography and etching techniques have resulted in reduction of minimum feature size and, at the same time, advances in materials technology have allowed integration of more devices for a given area. Consequently, electrical interconnections begin to play a more significant role in the limits of device and circuit performance [1]. The electrical characteristics of interconnects, namely their resistances, inductances, and capacitances must be carefully characterized in order to optimize circuit behavior [2].

Degradation of the signal integrity and speed due to coupling and stray capacitances has prompted the development of capacitance analysis programs [3]. One method for obtaining the capacitance characteristics for a particular cross-sectional geometry involves solving the two-dimensional Dirichlet problem for Laplace's equation,

$$\nabla \cdot [\varepsilon(x,y)\nabla V(x,y)] = 0, \tag{1}$$

where the electric potential $V(x,y)$ is prescribed on the boundary of a given domain. Traditionally, this problem has been solved deterministically, either analytically for simple geometries exhibiting spatial symmetry or numerically for more complicated geometries. Due to the complexity of typical integrated circuit cross-sections numerical techniques are most commonly employed.

The two most common numerical techniques are the Finite Difference Method (FDM) and the Finite Element Method (FEM). The drawback of any deterministic technique is that in order to find the potential at some local point, the solution must be obtained globally. This is due to the very nature of deterministic numerical techniques in that the entire domain of interest is discretized: a mesh for the FDM technique and sub-regions (elements) for the FEM technique. In the FDM technique Laplace's equation is replaced by its difference equation equivalent and then either direct (matrix inversion) or iterative (relaxation) methods are employed to solve for the potential. In the FEM technique the solution of Laplace's equation is approximated by a simple function over each element. The global solution is then obtained by combining the solutions for the many elements. If the solution of the potential equation is required at only one point (or some limited number of points as in a capacitance calculation), then considerable amount of time is wasted in calculating potentials at points that are of little or no interest.

An alternate, less common method for solving Laplace's equation employs a statistical approach [4], [5]. This approach allows a solution to be found at any desired point without knowing the solution nearby. Therefore, statistical methods become ideal for capacitance calculations where only a select number of points are important.

The object of this paper is not to calculate capacitances, but to present an improved algorithm for solving the multi-dielectric Dirichlet problem that can be embedded in a stochastic capacitance extraction algorithm. Specifically, we show how existing algorithms for the multi-dielectric Dirichlet problem can be improved by using statistically calculated Green's functions.

In Section II we begin our presentation by discussing how random-walk algorithms for the Dirichlet problem arise from statistical evaluation of integrals. We cover in this discussion both the single-dielectric and multi-dielectric cases; and we outline the random-walk algorithm for both cases. In Section III an improved algorithm for the multi-dielectric problem is presented and discussed. In Section IV, numerical results for our improved algorithm are compared with the standard floating-random-walk algorithm for two different parallel-plate geometries. Lastly, in Section V we present some discussion and conclusions.

II. Floating-Random-Walk Algorithm

The floating-random-walk algorithm (FRWA) has been presented in detail elsewhere [6]–[8]. Here we will review the essential principles behind the FRWA since it provides a motivation for generating an improved multi-dielectric algorithm.

Refer to Fig. 1, where over the circumference of a unit circle we have prescribed some arbitrary potential $V(\phi)$. The quantity ϕ measures the polar angle and we assume a

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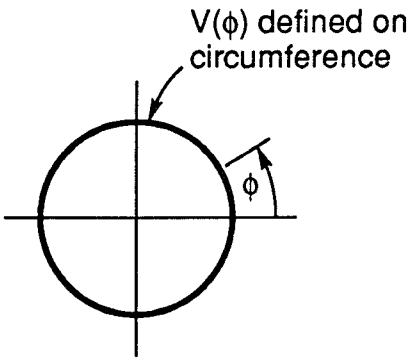

Fig. 1. Unit circle enclosing a single dielectric domain.

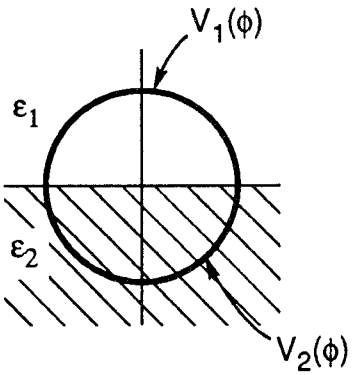

Fig. 2. Unit circle spanning a multi-dielectric domain with diameter on dielectric interface.

homogeneous medium with dielectric constant ε. To calculate the potential at the center of the circle, we use the Poisson integral formula [9] to get

$$V(0) = \int_0^{2\pi} d\phi V(\phi) p(\phi), \tag{2}$$

in which

$$p(\phi) = \frac{1}{2\pi}. \tag{3}$$

It has been shown [8] that

$$V(0) = \int_0^{2\pi} d\phi V(\phi) p(\phi) = \frac{1}{N} \sum_{i=1}^{N} V(\Phi_i), \tag{4}$$

where Φ_i is a random number whose probability density function (PDF) is $p(\phi)$. In other words, the potential at the center of the circle can be determined using the following statistical procedure: Pick random numbers $\Phi_i (i = 1, \cdots, N)$ whose PDF is $p(\phi)$ and evaluate $V(\Phi_i)$. Take the average of N such values of V to obtain the potential at the center. Note, that for this homogeneous case, the potential at the center of the circle is independent of the dielectric constant.

Now, refer to Fig. 2. The domain is inhomogeneous possessing dielectric constants ε_1 and ε_2. In this situation the dielectric interface lies on the diameter of the unit circle. The center potential is now given by [10].

$$V(0) = \left(\frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2}\right)\left(\frac{1}{\pi}\right)\int_0^{\pi} d\phi V_1(\phi) + \left(\frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2}\right)\left(\frac{1}{\pi}\right)\int_{\pi}^{2\pi} d\phi V_2(\phi). \tag{5}$$

When the two dielectrics are the same ($\varepsilon_1 = \varepsilon_2$) (5) reduces to

$$V(0) = \frac{1}{2\pi}\int_0^{2\pi} d\phi V(\phi), \tag{6}$$

as required. We defer the statistical interpretation of (5) until discussion of our multi-dielectric random-walk algorithm.

A. Single-Dielectric Case

At this point we briefly review the FRWA for the single dielectric geometry of Fig. 3. The boundary is assumed to have some prescribed voltage $V(s)$. The parameter s measures boundary length. We will statistically evaluate the potential

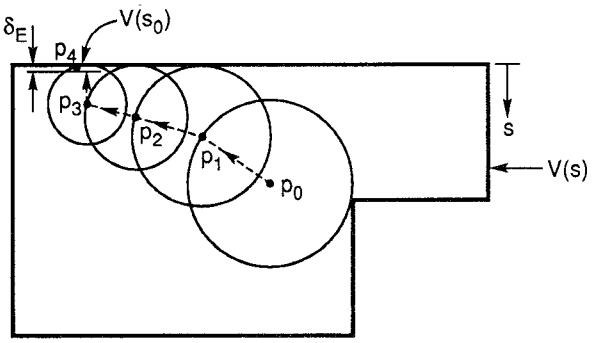

Fig. 3. Single-dielectric geometry illustrating the FRWA.

at some arbitrary point p_0. We begin by drawing the largest possible circle with radius r_0 centered at p_0 that does not cross the boundary. This we term a "maximal circle." In accordance with (4), we choose a polar angle randomly that is uniformly distributed on $[0, 2\pi]$. This angle specifies a new point p_1 on the circle circumference. Again, a maximal circle, this time with radius r_1, is drawn. A uniformly distributed random angle is chosen to specify a new point p_2 on the new circumference. This procedure is repeated until the point lies within some small distance, say δ_E, of an electrode. At this point the random walk terminates and is "captured" by the electrode. We take as the reward the value of the potential of the electrode nearest the termination point, in this example, $V(s_0)$.

If the above procedure is repeated N times, the potential at the point p_0 will be the average reward, the sum of all the rewards divided by N. As N increases the calculated result becomes more accurate with a statistical error $\sim \frac{1}{\sqrt{N}}$ [8].

B. Multi-Dielectric Case

Some modifications, however, are required to handle the multi-dielectric problem. Note Fig. 4, where the structure consists of two different dielectrics ε_1 and ε_2. Suppose, again, we are to find the potential at the point p_0. We begin by drawing a maximal circle, in this case limited by the distance to the nearest electrode or dielectric interface [8]. Therefore, the maximal circle will usually be smaller than the maximal circle in the single-dielectric case. New points are randomly chosen as before except that now the random walk can be captured by either the outer boundary or the dielectric interface.

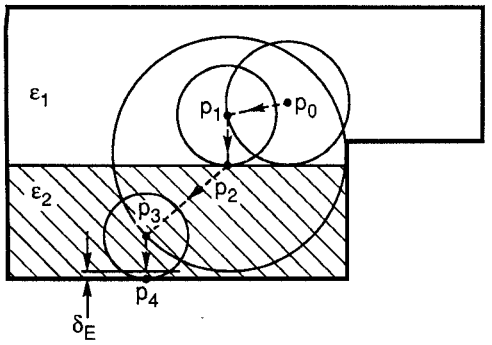

Fig. 4. Multi-dielectric geometry illustrating the FRWA.

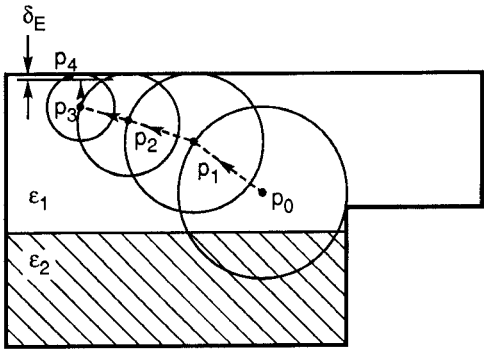

Fig. 5. Multi-dielectric geometry illustrating improved FRWA.

If the random walk is captured by the boundary, the walk is terminated and the reward is the value of the potential at the boundary electrode. If the walk is captured by the dielectric interface as shown in Fig. 4 (p_2), then a maximal circle is drawn about the interface termination point. This is reminiscent of Fig. 2 where (5) applies. Accordingly the walk must end upon the circumference of the circle in medium ε_1 or on the circumference in medium ε_2. Which circumference is determined by the coefficients of the two terms in (5). The probability of transition to dielectric ε_1 is therefore $\varepsilon_1/(\varepsilon_1 + \varepsilon_2)$, and the probability of transition to dielectric ε_2 is $\varepsilon_2/(\varepsilon_1 + \varepsilon_2)$. The specific polar angle is found on the respective semi-circle in the usual way. For example, suppose the next transition is in ε_1, then we choose an angle between $[0, \pi]$ in a uniform manner. If, on the other hand, the next transition is in ε_2 (as shown for p_3), then we choose an angle between $[\pi, 2\pi]$ with uniform PDF. This scheme requires the generation of two random numbers, one to determine in which dielectric region the transition is to take place, and another to determine the associated polar angle. As expected, the random walk terminates when encountering a boundary to within a distance δ_E.

Repeating the above procedure N times, the potential at the point p_0 will be the average reward, calculated as the sum of all the rewards divided by N. Observe that it is possible for the random walk to make several transitions at the dielectric interface before being captured at the boundary.

III. Improved Algorithm

We present an improved algorithm for the multi-dielectric problem. Fig. 5 shows the point p_0 where the potential is to be found. The maximal circle is drawn *only* to the nearest boundary, the dielectric interface being ignored. Fig. 6 shows the first maximal circle depicted in Fig. 5. Clearly, (5) no longer holds because the dielectric interface is not a circle diameter. Unfortunately there is no simple analytical expression describing the transition probability to medium ε_1 or ε_2. In fact, these transition probabilities are a function of the normalized distance d/a, and the dielectric constants as shown in Fig. 6. Here, a is the radius of the circle and $|d|$ is the normal distance form the dielectric interface to the center of the circle. The sign for d is $+/-$ depending on whether the dielectric interface is in the upper/lower half of the circle.

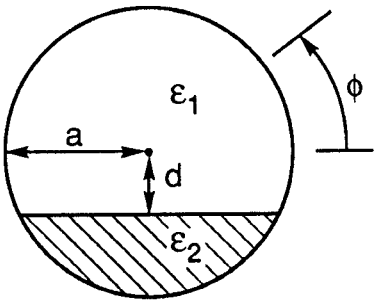

Fig. 6. Unit circle spanning multi-dielectric medium with diameter not on a dielectric interface.

We have resorted to a numerical evaluation of the transition probabilities for the structure of Fig. 6 as part of the improved FRWA for the multi-dielectric problem described here. As opposed to receiving a reward equal to the potential on the circumference, the point at which the random walk terminated (to within a distance δ_E) was recorded.

For a series of fixed d/a and $\varepsilon_2/\varepsilon_1$ ratios, 10^5 random walks were performed. Fig. 7 plots the numerically calculated transition probability density function for the case $d/a = -0.5, \varepsilon_1 = 1.0$ and $\varepsilon_2 = 3.9$, as a function of polar angle ϕ. These transition probability density functions are essentially surface Green's functions for this problem [11], [12]. By integrating the transition probability density function, one obtains the cumulative distribution function (CDF). The CDF enables one to obtain random numbers with the corresponding PDF using uniformly distributed random numbers. We have obtained Green's functions for d/a ranging from -0.9 to $+0.9$ in increments of 0.1 and $\varepsilon_2/\varepsilon_1 = 3.9$. Their corresponding CDFs have been stored in computer memory to be used as look-up tables.

Our improved multi-dielectric algorithm can now be described as follows. Referring back to Fig. 5, we start the random walk at point p_0 by drawing a maximal circle r_0 to the nearest outer boundary. Next, the distance to the dielectric interface is computed and normalized by the radius of the maximal circle. This yields the distance d/a which is rounded to the nearest d/a in the Green's function look-up table. By generating a random number with a suitable PDF (an example of which is shown in Fig. 7 for $d/a = -0.5$) the polar angle for the next transition is immediately determined. The random walk is continued in this manner until captured by the outer

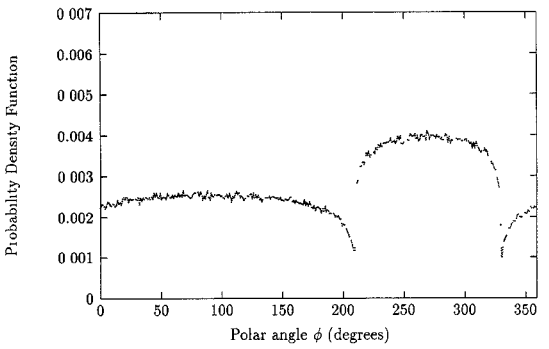

Fig. 7. The numerically calculated PDF for the geometry in Fig. 6, where $y = -0.5, \varepsilon_1 = 1.0$, and $\varepsilon_2 = 3.9$.

TABLE I
RESULTS OF POTENTIAL CALCULATION FOR OLD AND NEW METHODS AND COMPARISON WITH ANALYTICAL VALUES FOR STANDARD TWO -DIMENSIONAL PARALLEL-PLATE GEOMETRY OF FIG. 8.

y Position	*Analytical Value (V)*	*Potential Due to Old Method (V)*	*Percent Error*	*Potential Due to New Method (V)*	*Percent Error*
1.0	0.408	0.403 ± 0.022	1.2	0.413 ± 0.019	1.2
2.0	0.816	0.818 ± 0.026	0.2	0.845 ± 0.028	3.6
3.0	1.224	1.226 ± 0.035	0.2	1.257 ± 0.037	2.7
4.0	1.663	1.679 ± 0.039	2.8	1.608 ± 0.031	1.5
5.0	2.041	2.045 ± 0.038	0.2	2.095 ± 0.045	2.6
6.0	3.633	3.777 ± 0.046	4.0	3.628 ± 0.049	0.1
7.0	5.224	5.262 ± 0.041	0.7	5.225 ± 0.050	0.0
8.0	6 816	6.775 ± 0.048	0.6	6.808 ± 0.051	0.1
9.0	8.408	8.395 ± 0.035	0.2	8.429 ± 0.037	0.2

boundary. It is possible for the maximal circle not to intersect the dielectric interface in which case the next point is chosen in accordance with the usual FRWA for a single dielectric.

The advantage of this improved algorithm is that "bouncing" back and forth at the dielectric interface is minimized since the random walk can essentially "pass," unimpeded, through a dielectric interface. A faster algorithm thereby results.

IV. NUMERICAL RESULTS

We compare the usual FRWA with our improved version for two parallel-plate geometries. Fig. 8 shows a simple parallel-plate geometry with the dielectric interface half-way in between. The lengths of the plates and interface were chosen large enough so that fringing effects could be neglected. The upper region has a dielectric constant $\varepsilon_1 = 1.0$ and the lower region has a dielectric constant $\varepsilon_2 = 3.9$. The upper electrode is fixed at 10.0 volts and the lower electrode is fixed at 0.0 volts. The potential is calculated at nine different points. The x coordinate of all the points is fixed at 50 units and the y coordinate of the nine points range from 1 to 9 units. Table I lists the potential as a function of y. The results for the conventional algorithm and new algorithm are compared to exact analytical values. We present the 95% confidence intervals for the simulated data. Statistically, there is no loss of accuracy with the improved method when compared to the conventional method.

Fig. 9 shows the difference in execution time between the two algorithms for different values of y. The execution time for the new method does not include the time required to initially

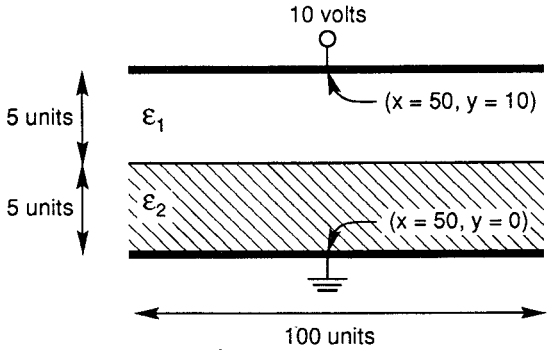

Fig. 8. Geometry for parallel-plate capacitor structure with two dielectrics.

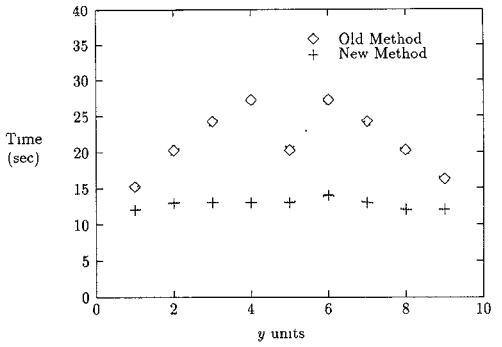

Fig. 9. Plot of execution time versus position for the old and new methods.

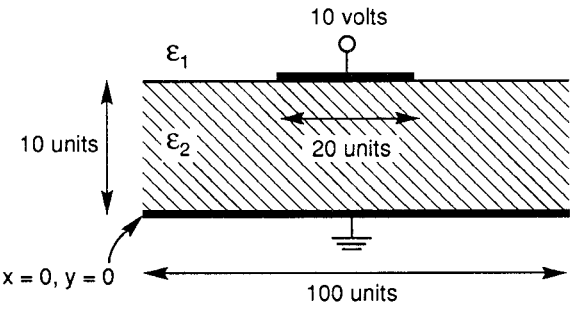

Fig. 10. Geometry for micro-strip structure with two dielectrics.

load the table in memory (on the order of 1–2 seconds). Because random walks in the conventional method are captured by the dielectric interface before passage, numerous reflections about the interface occur; consequently execution is slower. We observe this phenomenon, in particular, when the initial point of the random walk lies near to the dielectric interface ($y = 5.0$). Note as well, execution time for the improved method remains more or less constant with y.

Fig. 10 shows the micro-strip geometry for which no analytical solution of the potential exists. The finite size of the top electrode causes important fringing effects. Between the two electrodes the medium has dielectric constant $\varepsilon_2 = 3.9$, and above the top electrode is vacuum with dielectric constant $\varepsilon_1 = 1.0$. The potential on the top electrode is 10.0 volts and the bottom electrode is grounded at 0.0 volts. The potential was calculated at nine different points that are identified by the coordinates with respect to the origin as shown in Fig. 10.

TABLE II
RESULTS OF POTENTIAL CALCULATION FOR OLD AND NEW METHODS FOR TWO- DIMENSIONAL MICRO -STRIP GEOMETRY OF FIG . 10.

Position x, y	*Potential Due to Old Method (V)*	*Time of Execution in Seconds*	*Potential Due to New Method (V)*	*Time of Execution in Seconds*
50.0,15.0	7.707 ± 0.045	26	7.791 ± 0.043	17
55.0,15.0	7.495 ± 0.040	28	7.525 ± 0.044	17
60.0,15.0	6.108 ± 0.046	36	6.196 ± 0.042	18
65.0,15.0	4.039 ± 0.047	42	4.198 ± 0.053	18
65.0,10.0	3.460 ± 0.045	34	3.597 ± 0.046	16
65.0,5.0	2.154 ± 0.039	28	2.177 ± 0.034	15
60.0,5.0	3.661 ± 0.046	22	3.729 ± 0.048	14
55.0,5.0	4.698 ± 0.050	16	4.702 ± 0.045	13
50.0,5.0	4.863 ± 0.048	15	4.904 ± 0.050	14

Table II shows the calculated potential at the various points using the conventional and improved methods. The 95% confidence intervals for the potentials are given. Also shown is the execution time for the two methods. The improved method is faster than the conventional method every point. The explanation is similar to that given for the earlier parallel-plate example.

V. CONCLUSIONS

The FRWA applied to two-dimensional, multi-dielectric domains subject to Dirichlet conditions is ideally suited for problems where the potential needs to be evaluated at only a select number of points. Existing algorithms for solving the multi-dielectric algorithm are inefficient and, hence, slow. We have presented an improved algorithm, which, because of its greater efficiency, is about two times faster than the existing FRWA. This speed-up is achieved by using pre-calculated transition probabilities (or Green's functions) for some arbitrary two-dimensional problem. Similar pre-calculations can be done for more dielectrics if necessary. The Green's functions need be calculated only once for some specific set of dielectric constants. Once calculated, they can be used for any geometry containing the same dielectric constants.

The speed-up in the performance becomes especially useful when the potential is being calculated at many points that are near the dielectric interface. This feature, for example, can be exploited to a great degree in a recently developed FRWA that calculates capacitances between complex integrated-circuit interconnects [13].

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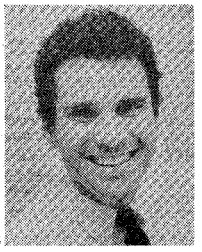

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Dr. Le Coz has received a variety of awards and honors including a Digital Corporation Fellowship; and has been a Summer-Faculty Fellow at the Sandia National Laboratories and at the Institute for Mathematics and Applications.