Numerical Characterization of Multi-Dielectric Green’s Function for Floating Random Walk Based Capacitance Extraction

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Abstract
The floating random walk (FRW) algorithm has several advantages for extracting interconnect capacitance. However, for multi-layer dielectrics in VLSI technology, the efficiency of FRW algorithm would be degraded due to the frequent stop of walk at dielectric interface. In this paper, an approach is proposed to calculate multi-dielectric Green’s function, which is utilized to enable hops across dielectric interface in the FRW. Numerical results show that the proposed approach is about 4X faster than an existing method, and brings several times speedup to the FRW-based capacitance extraction for actual multi-dielectric interconnect structures.

1. Introduction
As the feature size decreases and the number of transistors increases, interconnect capacitance has a growing impact on circuit performance. Therefore, effective algorithms to extract the capacitances of interconnect conductors are crucial in the design of high performance integrated circuits. Traditional deterministic algorithms, such as boundary element method with fast multi-pole acceleration [1], are fast and accurate, but not scalable to large structure due to the large demand of computational time or the bottleneck of memory usage.

In 1992, a 2-D floating random walk (FRW) algorithm was proposed to extract the interconnect capacitance [2]. The FRW algorithm is based on the Monte Carlo method for integral calculation, and converts the procedure of capacitance extraction to the random walks in dielectric space. It has the advantages of lower memory usage, more scalability for large structures and tunable accuracy, if compared with the deterministic methods [1]. The FRW algorithm has evolved to a commercial capacitance solver (QuickCap of Magma Inc.) for the design and analysis of VLSI circuits [4], and has also some recent advances for variation-aware capacitance extraction [3]. However, there is little literature which reveals the algorithm details of the 3-D FRW for multi-dielectric capacitance extraction. Recently, we’ve developed the technique of FRW to handle multi-dielectric structure, with the introduction of sphere transition domain [5].

However, while extracting the actual VLSI interconnects embedded in five to ten layers of dielectrics, the efficiency of FRW algorithm would be largely lost. The major reason is that the walk stops frequently at the dielectric interface, causing large increase of hops.

To improve the efficiency of FRW algorithm for multi-dielectric problem, an approach is constructing the random walk’s transition domain across dielectric interface. Due to the lack of analytical solution of the Laplace equation within a multi-dielectric domain, numerical technique is needed to generate the Green’s function for FRW [6]. This idea was employed by the FRW-based capacitance extractor CAPEM [7]. However, the techniques in CAPEM are not published yet.

In this paper, the techniques based on finite difference method (FDM) are proposed to characterize the multi-dielectric Green’s function for cubic transition domain. Utilizing the multi-dielectric Green’s function, the efficiency of FRW in [5] is improved remarkably, with acceptable memory overhead. The FDM-based technique is also compared with CAPEM, and the results show that our pre-characterization procedure is several times faster than the latter, while preserving same accuracy.

2. 3-D floating random walk algorithm for capacitance extraction
In the FRW algorithm, the fundamental formula is:

\[ \Phi(r) = \int_S P(r,r^{(1)})\Phi(r^{(1)})dr^{(1)} \]  

(1)

where \( \Phi(r) \) is the electric potential on point \( r \), \( S \) is a closed surface surrounding \( r \). \( P(r,r^{(1)}) \) is called the Green’s function. If \( S \) is the surface of a homogeneous cube or sphere centered at \( r \), \( P(r,r^{(1)}) \) only depends on the relative position of \( r^{(1)} \) with respect to \( r \), and can be regarded as the probability density function (PDF) for selecting a random point on \( S \). In this sense, \( \Phi(r) \) can be estimated by \( \Phi(r^{(1)}) \), if sufficient large number of random samples are evaluated. In [2, 4], the Green’s function for the cubic surface is derived analytically. And, the corresponding discrete probabilities for small pieces of cube surface are pre-computed, which forms the basis for an efficient FRW algorithm.

For the multi-conductor system within a single dielectric, (1) can be converted to a nested integral

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formula:
\[ \Phi(r) = \oint_{G_i} p^{(i)}(r, r^{(1)}) dr^{(1)} + \oint_{G_j} p^{(2)}(r^{(1)}, r^{(2)}) dr^{(2)} + \cdots + \oint_{G_k} p^{(k)}(\mathbf{r}^{(k)}, \mathbf{r}^{(k+1)}) \Phi(\mathbf{r}^{(k+1)}) d\mathbf{r}^{(k+1)} \]  
(2)

where \( S^{(i)} \), \( i = 1, \ldots, k + 1 \) is the \( i \)th cubic surface with center \( r^{(i)} \). \( p^{(i)}, i = 1, \ldots, k + 1 \), are the Green’s functions relating the potentials at \( r^{(i-1)} \) and \( r^{(i)} \). Once the potentials (voltages) on conductors are known, according to (2), the potential at \( r \) can be calculated with the following floating random walk procedure. Firstly, a maximum homogeneous cube centered at \( r \) is constructed, and a point \( r^{(1)} \) is randomly selected on the cube surface \( S^{(1)} \) according to the discrete probabilities resulted from the \( p^{(1)} \) function. If \( \Phi(\mathbf{r}^{(1)}) \) is known (e.g., \( r^{(1)} \) is on conductor surface), we can get an estimation of \( \Phi(\mathbf{r}) \). Otherwise, another cube centered at \( r^{(1)} \) is constructed similarly, and \( r^{(2)} \) is then randomly picked on \( S^{(2)} \). These steps are repeated until \( r^{(k+1)} \) is on conductor surface or remote from conductors, such that \( \Phi(\mathbf{r}^{(k+1)}) \) is known and becomes an estimation of \( \Phi(\mathbf{r}) \). This procedure is called a walk, for which the major cost is the geometric operation, since the probabilities are calculated in advance. After performing many walks, the mean value of these estimations becomes a fairly accurate \( \Phi(\mathbf{r}) \).

For extracting capacitances, the relationship between conductor charge and conductor potential is needed. So, a Gaussian surface \( G_i \) is constructed to enclose conductor \( i \), and according to the Gauss theorem,

\[ q_i = \oint_{G_i} D(r) \cdot \mathbf{n}(r) dr = \oint_{G_i} F(r)(-\nabla \Phi(r)) \cdot \mathbf{n}(r) dr \]  
(3)

where \( q_i \) is the charge on conductor \( i \), and \( F(r) \) is the dielectric permittivity at point \( r \). Substituting (2) into (3), we get:

\[ q_i = \oint_{G_i} F(r) g \oint_{S^{(i)}} \omega p^{(1)}(r, r^{(1)}) \Phi(\mathbf{r}^{(1)}) dr^{(1)} \]  
(4)

where

\[ \omega = -\nabla \cdot p^{(1)}(r, r^{(1)}) \cdot \mathbf{n}(r) g \]  
(5)

is called the weight value and constant \( g \) satisfies \( \oint_{G_i} F(r) g dr = 1 \). Now, the second integral in (4) can be calculated with the above FRW algorithm for potential, except for the extra calculation of \( \omega \). Similarly, the first integral in (4) also suggests a procedure of selecting points on \( G_i \) randomly. This results in a FRW algorithm for capacitance extraction [2-4].

In [5], the situation where there are multiple dielectric regions is considered. Since the above FRW algorithm relies on that the cube for point transition is in a single dielectric, a sphere transition domain is introduced to continue the walk stopped at dielectric interface. The techniques of selecting point on sphere surface and constructing transition domains are presented in [5]. The FRW algorithm for capacitance extraction with multiple dielectrics is illustrated in Fig. 1(a), and described as the following Algorithm 1.

**Algorithm 1 FRW for multi-dielectric problem**

1. Load the pre-computed probabilities and weight values for single-dielectric cubic transition domain;
2. Construct the Gaussian surface enclosing the master conductor \( i \);
3. \( C_{ij} = 0 \); \( npath = 0 \);
4. Repeat
5. \( npath = npath + 1 \);
6. Pick a point \( r^{(0)} \) on Gaussian surface, and then generate a single-dielectric cubic transition domain \( T \) centered at it; pick a point \( r^{(1)} \) on the surface of \( T \), and then calculate the weight value \( \omega \);
7. Until the stopping criterion is met

**3. Numerical characterization of multi-layer Green’s functions**

**3.1 Basic idea**

In this section, the technique for numerical characterization of multi-layer Green’s function is proposed. The Green’s function describes the relationship between the center point and boundary points of a transition domain, from the view point of potential. In FRW, this guides the selection of random point on boundary of transition domain. If the Green’s function, i.e., the probabilities, for a cube transition domain involving multiple dielectrics is available, the walk will be able to cross dielectric interface, resulting in fast completion of the FRW. In Fig. 1(b), there are two such cube domains, and the number of hops is therefore reduced. With the multi-layer Green’s function, the step 8 in Algorithm 1 can be revised; we can always construct the cube transition domain in the dielectric space.

In this work, we consider the unit-size cube domain including two dielectric layers, and derive the Green’s
function numerically. In each homogeneous sub-domain, the Laplace equation holds:

$$\nabla^2 \Phi = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0 \quad (6)$$

The whole problem domain is a cube including two dielectrics (as shown in Fig. 2). At the interface of dielectrics, there is the continuous condition:

$$\epsilon^+ \frac{\partial \Phi}{\partial x}(r) = \epsilon^- \frac{\partial \Phi}{\partial x}(r) \quad (7)$$

where $\epsilon^+$ and $\epsilon^-$ are the permittivities of up and down dielectric layers, respectively. The problem is to solve equations (6), (7), and express $\Phi(\tau_c)$ with the potentials on the boundary, where $\tau_c$ is the center of the cube.

![Figure 2 The cubic transition domain for calculating the Green's function (2D cross-section view)](image)

### 3.2 Calculating the Green's function with finite difference method

The finite difference method (FDM) can be used to solve the Laplace equation with multi-dielectric region. After discretization, the following matrix equation is got:

$$\begin{bmatrix} E_{11} & E_{12} & E_{13} \\ 0 & I_2 & 0 \\ E_{31} & 0 & D_{33} \\ \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \end{bmatrix} = \begin{bmatrix} f_1 \\ 0 \\ 0 \\ \end{bmatrix} \quad (8)$$

where $\Phi_1$, $\Phi_2$, and $\Phi_3$ are the potential unknowns on inner grid points, boundary, and interface respectively; $f_B$ is the boundary potentials, which may be given as the Dirichlet boundary condition. The third row of (8) is derived from (7), so that $D_{33}$ is a diagonal matrix. Also note that $I_2$ is an identity matrix.

We then have:

$$\Phi_k = -(E_{11} - E_{13} D_{33} E_{13})^{-1} E_{12} f_B \quad (9)$$

It expresses the relationship between the inner points and the boundary points. Suppose the center of the cube is the kth grid point of FDM. Then,$$\Phi_k = \epsilon^+ \frac{\partial \Phi}{\partial x}(r) = -(E_{11} - E_{13} D_{33} E_{13})^{-1} E_{12} f_B \quad (10)$$

The row vector

$$P_k = -(E_{11} - E_{13} D_{33} E_{13})^{-1} E_{12}$$

represents the discrete probabilities for transition from the center point to the boundary panels, and is what we want. It can be proved that $\|P_k\| = 1$.

The above deduction assumes that both the center point and dielectric interface are adapted to the FDM grid. This requests that each edge of the domain is divided into $2N+1$ segments, and one unknown is attached to each grid cell's center. They form the $\Phi_k$ for inner grid points. For each boundary panels, its center point is attached by an unknown, which forms $\Phi_B$. Extra unknowns $\Phi_F$ are defined on the interface surface.

Note that the height of interface $Z_i$ has the value of $1/2N+1$, $2/2N+1$, ..., or $2N/2N+1$ (see Fig. 2).

Different finite difference schemes are used to generate the coefficient matrix blocks in (8). For the inner grid point, the standard seven-point differential scheme is used (see Fig. 3(a)). For the grid point near boundary as shown in Fig. 3(b), its distance to boundary face is only $h$ (we assume the inner grid size is $2h$). The Lagrange interpolation is used to derive the differential scheme. For example, we approximate the $z$-direction derivative for the point in Fig. 3(b) with:

$$\frac{\partial^2 \Phi}{\partial z^2}(r) = \frac{2u_0 - u_1 + u_2}{6h^2} \quad (12)$$

Here $u$ denotes the potential on grid point. For the point on interface, another finite difference equation is needed to approximate (7). In order to be consistent with the scheme for (6), the formula with second-order accuracy is required. As shown in Fig. 3(c), on each side of the interface the Lagrange interpolation with three points is used to derive the approximate formula for $\frac{\partial \Phi}{\partial x}(r)$ or $\frac{\partial \Phi}{\partial y}(r)$. Finally, we get the following difference equation for the example in Fig. 3(c):

$$\epsilon^+ \frac{8u_0 - 9u_1 + u_2}{6h} = \epsilon^- \frac{8u_0 - 9u_1 + u_2}{6h} \quad (13)$$

With this formula, the severe discontinuous problem for generated Green’s function solutions can be avoided.

![Figure 3. Illustration of finite difference schemes for: (a) inner grid point, (b) grid point near boundary, (c) point on interface](image)

In the FDM solution, the height of interface $Z_i$ cannot be $1/2$, which omits an important situation like the cube (1) in Fig. 1(b). The special treatment should be taken. As shown in Fig. 4(a), which is a side view, the cube edge should be divided into even segments, so that there is no boundary panel across the interface. Therefore, the center point is not an inner grid point. As shown in Fig. 4(b), the potential of center point can be approximated by its eight neighbors. By modifying (11), an efficient approach is found to calculate the discrete
probabilities for the transition cube whose dielectric interface is at height 1/2. Due to the limit of space, its detail is omitted here.

3.3 Utilizing the numerical Green’s function
The multi-layer Green’s function can be pre-computed for all possible \((\varepsilon^+, \varepsilon^-)\) pairs. For each pair of \((\varepsilon^+, \varepsilon^-)\), a suitable value of segment number \(2N+1\) is assumed, which corresponds to \(2N\) different interface positions and thus \(2N\) Green’s function (GF) tables. An extra GF table is generated for the interface at height 1/2.

While running the FRW algorithm for capacitance extraction, the above GF tables are loaded from disk files. For each hop the transition cube is firstly maximized, and then might be cut if it crosses more than two dielectrics. For a cube including only two dielectric layers, its size may also be adjusted to match its height of interface to those in the GF tables. This is performed by shrinking its size, so as to minimize the numerical error induced by the GF tables.

4. Numerical Results
The method for calculating the Green’s function is implemented in MATLAB, using the functions for sparse matrix. And, the results are used by a FRW program written in C++ [5]. All experiments are carried out on a Linux server with Intel E5620 2.40GHz Xeon CPU.

4.1 Accuracy validation of the Green’s function
Fig. 5 shows examples of numerical Green’s function on the faces of cube, where \(N=12\) is set. The picture in Fig. 5(a) is consistent with that of single-dielectric Green’s function [4], and the pictures in Fig. 5(b), (c) demonstrate that there is much larger probability to walk towards the dielectric with higher permittivity. An experiment setting two dielectrics the same permittivity is also carried out. The results show that our numerical Green’s function is the same as the single-dielectric Green’s function.

![Figure 5. The probability distribution on cube boundaries: top face (a), and side face with interface height of 1/5 (b), or 1/2 (c) (the relative permittivities are \(\varepsilon^- = 2.6\) and \(\varepsilon^+ = 5\))](image)

4.2 Efficiency comparison
The proposed method is compared with CAPEM [7], which is a binary-coded program. For different segment numbers \((2N+1)\) along one edge of the cube, the computational time of both programs for each GF table are given in Fig. 6. From this figure, we can see that our Matlab program is more efficient than CAPEM. If the segment number is 51, the former is about 4X faster than the latter.

![Figure 6. Computational time vs. segment number per edge](image)

To reveal the validity of the multi-layer Green’s function, two multi-dielectric interconnect structures are extracted with the FRW program. The first case has 5 dielectric layers, and 41 crossing metal wires in three layers. The second case has 9 layers of dielectrics and similar structure of wires as the first case. The GF tables with segment number 51 are used. Numerical results show that by utilizing the multi-layer Green’s function, the FRW program exhibits the speedup ratios of 1.9X and 2.7X, for the two cases respectively. The memory overhead for loading the GF tables is only about 21MB.

5. Summary
The technique based on FDM is proposed to characterize the two-layer Green’s function. It is utilized to enable the hop across dielectric interface in the FRW algorithm, thus improve the efficiency of capacitance extraction. Numerical results reveal that the proposed approach is several times faster than an existing method in CAPEM [7], and provides remarkable efficiency improvement for the FRW-based extraction of actual multi-dielectric interconnect structures.

References