A Statistical Algorithm for 3-D Capacitance Extraction

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***Abstract*—This letter deals with the problem of parasitic capacitance extraction in deep submicron layouts having general geometries. The here presented extraction method is based on the statistical floating random walk algorithm. It employs a suitable spherical Green function that, in a charge free region, relates the electrical field in the sphere center to the surface electrical potential.**

***Index Terms*—Capacitance measurement, Laplace equation.**

I. Introduction

THE determination of static electrical capacitances of conductors embedded in a three dimensional electrodes arrangement is an important and recurrent task for modeling modern ultra large scale integration (ULSI) circuits. In submicron layouts the parasitic capacitance of interconnects with respect to the substrate (ground plane) and neighboring conductors is one of the main causes that affect the signal delay and clock skew.

The extraction of the electrostatic capacitance is a well known problem that involves the solution of Laplace's equation for the electrical potential.

Among the possible techniques for solving the Laplace's equation, statistical methods based on the floating random walk (FRW) are particularly promising since they can efficiently handle very complex geometries.

A careful investigation of the influence of geometry complexity on the CPU time and memory occupation of FRW methods has been recently presented in [2] and compared to those of conventional finite-element and boundary element methods.

FRW was originally introduced by Royer for computing the electrical potential in a 3-D geometry [3] and was based on the employment of spherical surfaces. Iverson and Le Coz extended this method to the determination of the parasitic capacitance of an interconnect, basing it on the usage of cubic surfaces [4]. The advantage of employing cubic surfaces is that they better conform to the contour of Manhattan geometries, largely found in ICs layout.

As far as we know, a capacitance extraction method based on spherical Green function for the electrical field was never investigated before and constitutes the subject of this paper. This choice is based on the fact that ICs manufacturing technology is evolving toward non regular Manhattan shapes. The superior conform ability of cubes is greatly lost for these structures and there is no reason to approximate them with Manhattan ones if an efficient capacitance extraction method can be applied.

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There is another aspect for which FRW based on spheres is worth to be reconsidered: as it will be shown in the sequel, the probability function derived from spherical Green functions is directly invertible while those ones of cubes do not. As a consequence the FRW method based on sphere is straightforward ensuring high robustness and minimal memory occupation.

II. Mathematical Foundation

Let consider the 3-D solution of Laplace's equation for the electrical potential Φ subjected to the boundary Dirichlet conditions on the surface of a sphere. The problem is suitable for a description in spherical coordinates where r is the radius, θ the polar angle and ϕ the azimuth angle. The general expression of the electrical potential in the interior of the sphere is

$$\Phi(r,\theta,\phi)=\sum_{m=0}^{\infty}\sum_{n=0}^{m} C_m r^m[A_n\cos(n\phi)+B_n\sin(n\phi)]\cdot P_m^n(\cos\theta) \tag{1}$$

where $P_m^n(\cos\theta)$ are the Legendre polynomials [5]. It is possible to evaluate the partial derivative of the potential along the radial direction in the sphere center

$$\left.\frac{\partial\Phi}{\partial r}\right|_{r=0}=A_oC_1\cos(\theta)+A_1C_1\cos(\phi)\sin(\theta)+C_1B_1\sin(\phi)\sin(\theta). \tag{2}$$

By employing spherical to rectangular coordinate transformations $x=r\sin(\theta)\cos(\phi)$, $y=r\sin(\theta)\sin(\phi)$ and $z=r\cos(\theta)$ and the derivative chain rule, it is easy to show that

$$A_1C_1=\left.\frac{\partial\Phi}{\partial x}\right|_{r=0}=\Phi_x(0)=-E_x(0)$$
$$C_1B_1=\left.\frac{\partial\Phi}{\partial y}\right|_{r=0}=\Phi_y(0)=-E_y(0)$$
$$A_oC_1=\left.\frac{\partial\Phi}{\partial z}\right|_{r=0}=\Phi_z(0)=-E_z(0)$$

where $E_i(0)$ is the electrical field component along the ith axis. The coefficients in (1) are found by imposing the potential on the spherical surface of radius R be equal to a known $V(\theta,\phi)$ potential distribution. Exploiting the orthogonality properties of Legendre polynomials and sinusoidal functions, we find

$$\begin{aligned}\int_{-\pi}^{\pi}d\phi\int_0^{\pi}\Phi(R,\theta,\phi)(P_1^o)^2\sin(\theta)\,d\theta&=\int_{-\pi}^{\pi}d\phi\int_0^{\pi}RA_oC_1(P_1^o)^2\sin(\theta)\,d\theta\\&=\frac{4R\pi}{3}\Phi_z(0).\end{aligned} \tag{3}$$

By substituting $P_1^o = \cos(\theta)$ we obtain a weighted summation of the potential on the boundary

$$\Phi_z(0) = \frac{3}{2R} \int_{-\pi}^{\pi} \frac{1}{2\pi}\, d\phi \int_0^{\pi} V(\theta, \phi) \cos(\theta) \sin(\theta)\, d\theta \quad (4)$$

Similar expressions can be found for the other field components. If we define $\theta' = \pi - \theta$, the azimuth complementer angle, we have

$$\Phi_z(0) = \frac{3}{2R} \int_{-\pi}^{\pi} \frac{1}{2\pi} \left(\int_0^{\pi/2} V(\theta, \phi) \cos(\theta) \sin(\theta)\, d\theta - \int_0^{\pi/2} V(\theta', \phi) \cos(\theta') \sin(\theta')\, d\theta' \right) d\phi \quad (5)$$

which shows that potentials on the half-sphere surface with positive z coordinate give a positive contribution to the derivative of the potential in the sphere center, while potentials on the other half-sphere give a negative contribution. The numerical evaluation of the integral can be done with a statistical procedure: the weighting factor is the probability density function of θ and ϕ variables. If the electrical field along a generic direction $\vec{n}$ is desired, a local rectangular coordinate frame of reference is chosen with the z direction oriented as $\vec{n}$. In this reference the ϕ angle is distributed uniformly in the interval $[0, 2\pi]$ while θ and its complementer θ' are distributed in $[0, \pi/2]$ with the probability density $G_e^{(Sph)} = \sin(\theta) \cos(\theta)$, which is related to the cumulative probability function $1/2 \sin^2(\theta)$ that is simple and invertible. As a consequence the statistical evaluation of the electrical field can be done by directly generating the azimuth and polar angles $\phi = 2\pi I[0, 1]$; θ or $\theta' = \arcsin \sqrt{(I[0, 1])}$ where $I[0, 1]$ is a random number uniformly distributed between 0 and 1. Note that θ angle or its complementer are selected with equal probability. The electrical potential of the corresponding point on the spherical surface is multiplied by the factor $3/2R$, taken negative if $\theta < \pi/2$ or positive if $\theta' < \pi/2$, and stored in memory. Repeating many times this procedure and averaging results, the statistical estimation of the electrical field is obtained.

We note that the Green functions relating the electric field and the potential in the center of a cube to its surface potential distribution, here referred to as $G_e^{(Cube)}$ and $G_v^{(Cube)}$, have much more complicated expressions and in 3-D they require double infinite series summations. Therefore the corresponding cubic cumulative probability functions are not directly invertible.

III. Capacitance Computation

The structure we refer to is formed by N electrical conductors of possible different shapes in a 3-D domain. To determine the generic C_{ij} is necessary to compute the charge q_i induced on the ith electrode when the potential of the jth electrode is raised to one volt and the other electrodes are grounded. The induced charge is derived from the Gauss' law by evaluating the flux of the electrical displacement vector through a Gaussian surface G that surrounds the electrode $q_i = \varepsilon \int_G \vec{E} \cdot \vec{n}\, dG$. By means of the previously developed equations, we have

$$q_i = \varepsilon \frac{G}{N_s} \sum_{i=1}^{N_s} \left(\int \frac{1}{2\pi}\, d\phi_i \int V(\theta_i, \phi_i) \cos(\theta_i) \sin(\theta_i)\, d\theta_i \right) \quad (6)$$

where N_s is the number of random walks performed by the algorithm. The statistical evaluation of the above integral is composed of the following steps.

- Randomly select a point on the G surface with uniform probability.
- Get a sphere that does not intersect electrodes, with the maximum radius $R_{\max}$ and centered in the selected point.
- Pick a point on this sphere accordingly to the procedure described in the previous section and store the factor $1.5/R_{\max}$.
- From the last point start with a floating random walk until an electrode is reached [3]. An electrode is considered touched when the walking point is at a distance δ which is very small when compared with the electrode dimensions.

The potential of the reached electrode is multiplied by the previous $1.5/R_{\max}$ factor and stored in memory.

Some information on the extension to multidielectric structures can be found in [7].

IV. Numerical Results

In the first part of this section, we investigate the advantages and the drawbacks of the proposed FRW method by comparing it to the cubic based approach. We refer to very simple two–dimensional (2–D) examples that the reader can verify by himself. The $G_v^{(Sph)}$ Green function of the circle is a constant and a point selection on it is done with uniform probability. For the square, the $G_v^{(Cube)}$ function is reported in [4] and we have implemented it in a one-dimensional look-up table. In all the examples $\delta = 0.001$ μm is the tolerance chosen for the circle implementation while for the square each edge is discretized in 1000 pieces. With this choice, for an average square edge of 1 μm the discretization error introduced is comparable to the circle tolerance.

First, let us consider the 2-D symmetric Manhattan geometry of Fig. 1(a) and compute the average number of hops $W^{(Sph)}$ and $W^{(Cube)}$ that are required to reach one of the two electrodes starting from the point A and by moving on circles and on squares, respectively. It results $W^{(Sph)} = 10$ and $W^{(Cube)} = 4.3$, showing that in a regular Manhattan geometry, squares perform about two times better than circles.

Let us now consider the non symmetric Manhattan geometry shown in Fig. 1(b). Starting from point B, we obtain $W^{(Sph)} = 14$ and $W^{(Cube)} = 25$, while starting from C, $W^{(Sph)} = 12$ and $W^{(Cube)} = 10$. The better conform ability of square is largely lost for walks starting between not aligned conductors (B) and is only partially regained starting near the large electrode (C). From this example it follows that also in Manhattan geometries the more or less conform ability of square with respect to circles depends on the particular Gaussian surface from which the FRW is started.

Fig. 1(c) shows a non Manhattan geometry with non rectangular electrodes. In this case we obtain $W^{(Sph)} = 13$ and $W^{(Cube)} = 40$, starting from point D, $W^{(Sph)} = 13$ and $W^{(Cube)} = 20$, starting from E. Squares need the introduction of a δ tolerance in touching an electrode, similar to that of circles. While the average number of hops needed by circles is almost equal to those of previous cases, squares need much more

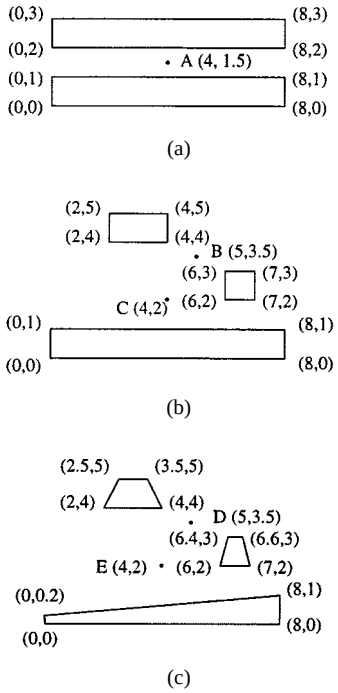

Fig. 1. (a) The 2-D symmetric Manhattan structure employed as benchmark, (b) the 2-D non symmetric Manhattan structure employed as benchmark, and (c) the 2-D non Manhattan structure employed as benchmark.

hopes to reach an electrode. Similar results are obtained if 3-D geometries are considered.

On our computer for the irregular geometries of industrial layouts, the proposed algorithm does 5000 walks/second in average and in general 1000–2000 walks are enough to estimate the capacitance of an interconnect with 5% relative error. Our experience with QuickCap [9] shows that it does less walks/second on the same layouts, but we are unable to definitely attribute this to the employment of cubes and not to a different structure of the program. To summarize our opinion is that an efficient FRW can be obtained in practice only through a careful choice of the Green function that governs hops and of the "clipping" algorithm that selects the maximum allowed step.

In the second part of this section, we compare the proposed FRW to FASTCAP that is based on the multi-pole acceleration algorithm [6].

Fig. 2 shows an interconnect with trapezoidal cross section on a ground plane in a uniform dielectric ($\epsilon_r = 4.2$). We extracted the total parasitic capacitance for several values L of the interconnect length with FASTCAP and with the here proposed FRW method ($\delta = 0.1$ nm). Table I shows the capacitance values evaluated by FASTCAP (**CF**) and by FRW (**CFRW**) with a chosen relative accuracy error of 1% and the corresponding CPU time, (**time-F**) and (**time-FRW**) respectively. All simulations were done on a PENTIUM III 500 Mhz.

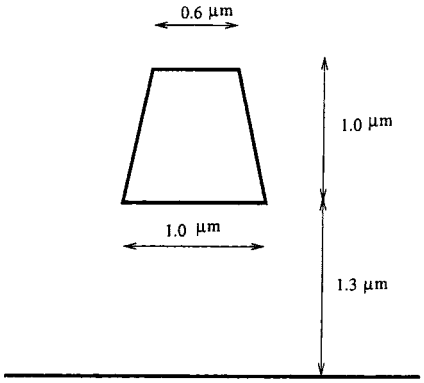

Fig. 2. Cross section with lengths of the interconnect.

TABLE I
CAPACITANCE VALUES EVALUATED BY FASTCAP (**CF**) AND BY FRW (**CFRW**)

L [μ m]	CF [fF]	time-F [sec]	CFRW [fF]	time-FRW [sec]
10	1.41	3.3	1.37	2.5
100	12.41	44.0	12.25	2.47
200	24.48	116.0	24.6	2.55

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