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Transient Simulations of Three-dimensional Integrated Circuit Interconnect using a Mixed Surface-Volume approach

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Abstract

It has recently been shown that the boundary-element method can be used to perform accurate cross-talk simulations of three-dimensional integrated circuit interconnect. However, the computational complexity grows as N^2, where N is the number of surface unknowns. Straightforward application of the fast-multipole algorithm reduces the computational complexity to order N, but produces magnified errors due to the ill-conditioning of the steady-state problem. We present a mixed surface-volume approach and prove that the formulation results in the exact steady-state solution, independent of the multipole approximations. Numerical experiments are presented to demonstrate the accuracy and efficiency of this technique. On a realistic example, the new method runs fifteen times faster than using dense-matrix iterative methods.

1 Introduction

When analyzing high-performance integrated circuit designs, it is well-known that the single lumped resistor-capacitor model of interconnect is insufficiently accurate. It has been suggested [1] that reasonably accurate electro-quasistatic, or transient interconnect, simulations could be performed by computing the time evolution of the electric field both inside and outside the conductors via a finite-difference discretization of Laplace's equation. More recently, a boundary-element approach [2] based on Green's theorem was proposed, which performs the caculation using the same surface discretization used for ordinary capacitance extraction, thereby avoiding the large, exterior domain mesh and computation. However, the latter approach generates dense matrix problems, which require $O(N^3)$ operations to solve directly, and at least $O(N^2)$ to solve iteratively, where N is the number of surface unknowns. Therefore it is necessary to accelerate such methods when solving large problems.

The direct application of the fast-multipole algorithm on the boundary-element formulation produces unacceptable results because the multipole errors are magnified by the ill-conditioning of the steady-state problem. In this paper, we introduce a mixed surface-volume approach, in which the finite-difference method is used to solve Laplace's equation *inside* the conductors, and the boundary-element method is used to couple all conductor surfaces globally. We then prove that this technique can be multipole-accelerated yet still produces the exact steady-state solution. Finally, we perform numerical experiments which show that the new formulation reduces the computational cost from $O(N^2)$ to $O(N)$.

2 Background

2.1 The Boundary-Element Formulation

For the transient interconnect problem, the system is assumed to be in the electro-quasistatic (EQS) regime. The scalar potential ψ satisfies

$$\nabla^2\psi(x) = 0, \qquad x \notin S, \tag{1}$$

which states that Laplace's equation holds everywhere except on conductor surfaces. Careful application of Green's theorem [2] results in an integral formulation

$$-4\pi\tau\frac{\partial\psi(x)}{\partial t} = 4\pi\psi(x) + \int_S \psi(x')\frac{\partial}{\partial n'}\frac{1}{\|x-x'\|}da' + \frac{1}{\sigma}\int_{S_{contact}}\frac{J_{external}(x')}{\|x-x'\|}da'. \tag{2}$$

Panel-based discretization leads to a system of equations

$$-4\pi\tau\frac{\partial}{\partial t}\Psi = (4\pi I + D)\Psi + PJ^{ext}, \tag{3}$$

where $\Psi \in \Re^N$, $J^{ext} \in \Re^N$ represent the panel potentials and externally supplied current densities, which are assumed to be uniform, $\tau = \epsilon/\sigma$ is the dielectric relaxation time of the conductors, and

$$P_{kl} = \frac{1}{a_l} \int_{panel_l} \frac{1}{||x' - x_k||} da', \tag{4}$$

$$D_{kl} = \int_{panel_l} \frac{\partial}{\partial n'} \frac{1}{||x' - x_k||} da'. \tag{5}$$

Suppose M of the N surface panels are connected to voltage contacts whose values are known *a priori*, then the potential vector Ψ has $(N - M)$ unknown entries. The vector of external current densities supplied by the contacts, $J^c \in \Re^M$, must also be computed so a total of N unknowns are generated. Equation (3) can be solved with the backward-Euler method, resulting in the matrix problem

$$\mathcal{H} \begin{pmatrix} \Psi^f \\ J^c \end{pmatrix}_{t=(m+1)h} = \frac{4\pi\tau}{h} \Psi_{t=mh} - \left(\frac{4\pi\tau}{h} I + 4\pi I + D \right) \begin{pmatrix} 0 \\ \Psi^c \end{pmatrix}_{t=(m+1)h}, \tag{6}$$

where, h is the timestep, $\Psi^c \in \Re^M$ and $\Psi^f \in \Re^{(N-M)}$ represent the elements of the potential vector associated with the contact and free panels, respectively. The $N \times N$ matrix, or linear operator, $\mathcal{H}$, is defined by its action on a vector

$$\mathcal{H} \begin{pmatrix} p \\ q \end{pmatrix} = \left(\frac{4\pi\tau}{h} I + 4\pi I + D \right) \begin{pmatrix} p \\ 0 \end{pmatrix} + P \begin{pmatrix} 0 \\ q \end{pmatrix}. \tag{7}$$

Since $\mathcal{H}$ is defined in terms of P and D, the unknowns can be interpreted as a distribution of sources and dipoles, with the panels associated with the elements of J^c acting as uniform sources (single layers), and the panels associated with Ψ^f acting as uniform dipoles (double layers).

2.2 Multipole Acceleration

Consider using a Krylov-subspace based iterative algorithm, such as GMRES [3], to solve (6) at each timestep. The k^{th} iteration of the GMRES algorithm requires computing the matrix-vector product $\mathcal{H}u^k$, where u^k is the k^{th} GMRES search direction. Since $\mathcal{H}$ dense, this costs N^2 operations. However, forming the matrix-vector product in this case is equivalent to computing potentials at N points due to N sources and dipoles, which can be computed approximately in order N operations using fast-multipole algorithms [4] [5] [6].

3 Effects of Ill-Conditioning

We found in our initial experiments that if the the multipole algorithm is applied directly to the pure boundary formulation in (6), the small errors from the multipole approximations are magnified due to the somewhat ill-conditioned steady-state problem.

L	2	4	8	16	32
voltage	0.997	0.985	0.938	0.822	0.248
κ	8.60	21.3	59.2	177	562

Table 1: Steady-state voltage and condition number versus wire length

Consider a rectangular wire with dimensions $L : 1 : 1$, which is connected to a unit-step voltage source at one end. The correct steady-state voltage at the opposite end is 1 volt. The values computed with the boundary-element method, accelerated by second-order multipole and local approximations, is given versus wire length in Table 1.

The errors introduced by the second-order multipole algorithm on the potential calculation, or equivalently the errors in the matrix-vector multiply, are typically 0.1-1%. However, the errors in the computed steady-state are much larger. This is because the steady-state problem is somewhat ill-conditioned, and this ill-conditioning magnifies the error [7]. The magnification factor for the steady-state solution is the steady-state matrix condition number, κ, and is given in Table 1. Note that the problem becomes more ill-conditioned as the wire length increases, resulting in larger steady-state errors.

4 The Mixed Surface-Volume Formulation

We derive here a mixed surface-volume formulation which can be multipole-accelerated without loss in solution accuracy. We begin with a pure boundary-element formulation similar to that in Section 2.1, and then we augment it with a volume-based finite-difference operator. Since Laplace's equation (1) holds both inside and outside of the conductors, all charges in the system reside on the conductor surfaces S. Therefore, the potential ψ is related to the conductor surface charge density, ρ_s, through the superposition integral,

$$\frac{\partial \psi(x)}{\partial t} = \int_S \frac{1}{4\pi\epsilon ||x - x'||} \frac{\partial \rho_s(x')}{\partial t} da'. \tag{8}$$

Charge conservation [8] at the surface yields the continuity condition $\frac{\partial \rho_s(x)}{\partial t} = J_{internal}(x) - J_{external}(x)$, where $J_{internal}$ and $J_{external}$ are the normal current densities taken just inside and just outside the conductor surface. The internal current obeys the constitutive relation $J_{internal}(x) = -\sigma \frac{\partial \psi}{\partial n}(x)$, where n is the outward normal to the surface S.

Combining (8) with charge conservation and the current constitutive relation, and noting that $J_{external} = 0$ for non-contact surfaces, we have

$$-4\pi\tau \frac{\partial \psi(x)}{\partial t} = \int_S \frac{1}{\|x - x'\|} \frac{\partial \psi}{\partial n'}(x')da' + \frac{1}{\sigma} \int_{S_{contact}} \frac{1}{\|x - x'\|} J_{external}(x')da'. \quad (9)$$

We now discretize the conductor surfaces into N panels as described in Section 2.1. The resulting matrix equation is

$$-4\pi\tau \frac{\partial}{\partial t}\Psi = P\Psi_n + PJ^{ext}, \quad (10)$$

where $\Psi_n \in \Re^N$ represents $(\frac{\partial \psi}{\partial n})$ at the N panels.

For each conductor in a given problem, if the potential is known on the entire surface, Laplace's equation can be solved for the *interior* domain to yield Ψ_n everywhere *just* inside the surface. Note that this is done *independently* for every conductor. Let $\mathcal{X}$ be defined such that

$$\mathcal{X}\Psi = \Psi_n, \quad (11)$$

and applying $\mathcal{H}$ implies solving the interior problems. Using (11) in (10) yields

$$-4\pi\tau \frac{\partial}{\partial t}\Psi = P(\mathcal{X}\Psi + J^{ext}). \quad (12)$$

Given Ψ at the surface nodes of a conductor, a finite-difference method can be used to solve for Ψ_n at each surface node, effectively applying $\mathcal{H}$.

As before, a fixed-timestep, backward-Euler method is used for time-integration. The resulting linear system is

$$\mathcal{H}' \begin{pmatrix} \Psi^f \\ J^c \end{pmatrix}_{t=(m+1)h} = \frac{4\pi\tau}{h}\Psi_{t=mh} - \left(\frac{4\pi\tau}{h}I + P\mathcal{X}\right) \begin{pmatrix} 0 \\ \Psi^c \end{pmatrix}_{t=(m+1)h}. \quad (13)$$

The new operator $\mathcal{H}'$ is defined by its action on a vector as

$$\mathcal{H}' \begin{pmatrix} p \\ q \end{pmatrix} = \frac{4\pi\tau}{h} \begin{pmatrix} p \\ 0 \end{pmatrix} + P\left\{\mathcal{X} \begin{pmatrix} p \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ q \end{pmatrix}\right\}. \quad (14)$$

In order to evaluate the costs of the volume-based computation, consider a typical transient interconnect problem, in which the self and mutual interactions of many relatively long and thin conductors are to be modeled. The action of the $\mathcal{X}$ operator then corresponds to solving a *block-diagonal* and *sparse* linear system. The dominant cost of the matrix-vector multiply in (14) comes from P, which is a *dense* matrix since it couples every panel to all panels on all conductors. But as described in Section 2.2, the fast-multipole algorithm can produce an approximate result in $O(N)$ operations. Therefore this technique can can be made very efficient.

The mixed surface-volume method provides an important guarantee on the solution accuracy. This is stated in the theorem below.

Theorem 4.1 *If the steady-state solution of (12) is such that the surface potential on each conductor is a constant, and none of the conductors is floating, then the solution computed by the mixed surface-volume method is exact, regardless of multipole approximation error and discretization error.*

Proof: Consider first the single conductor problem. From equation (12), the steady-state solution satisfies

$$\frac{\partial}{\partial t}\Psi = 0 = P(\mathcal{X}\Psi + J^{ext}). \quad (15)$$

From the theory of fractional Sobolev spaces, it can be shown that the potential coefficient matrix P is non-singular given a sufficiently fine discretization [9]. It then follows that $\mathcal{X}\Psi + J^{ext} = 0$ in the steady-state. In the finite-difference implementation of $\mathcal{X}$, this is equivalent to a resistor network connected to external voltage sources [1]. Assuming that all voltage sources are at 1 Volt, we get

$$\mathcal{X} \begin{pmatrix} \Psi^f \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ J^c \end{pmatrix} = 0. \quad (16)$$

In the equivalent resistor network picture, $(N - M)$ of the surface nodes are connected to unit-voltage sources, while the remaining M surface nodes are left open-circuited. Network analysis immediately yields $\Psi^f = 1$ and $J^c = 0$, the exact steady-state solution. For many-conductor problems, the same result holds since each conductor is treated independently by the $\mathcal{X}$ operator. □

Comparing (3) and (10), we see that in the limit as the mesh becomes very fine, $P\mathcal{X} \approx (4\pi I + D)$. Since $\Psi = \{1, 1, ..., 1\}$ implies $\mathcal{X}\Psi = 0$, $\mathcal{X}$ is a singular matrix. Thus both $(P\mathcal{X})$ and $(4\pi I + D)$ are singular.

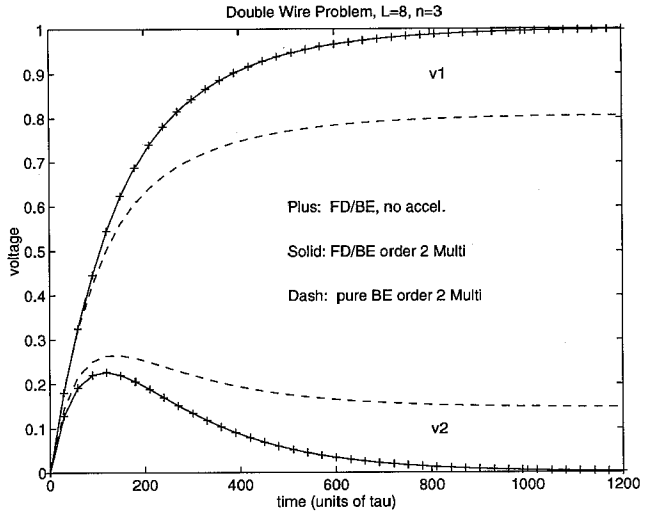

Figure 1: Multipole errors are magnified in the pure BE method but not in the mixed FD/BE method.

The surface-volume formulation essentially factorizes $(4\pi I + D)$ into the product of a singular $\mathcal{X}$ and a well-conditioned, non-singular P. When the action of P is multipole-accelerated in the mixed formulation, errors are introduced only in the capacitance matrix of the surface panels, which does not alter the physical character of the system. This error appears only during the transient, and will be shown experimentally to be small and independent of condition number. This is expected since approximations are made only on P, the well-conditioned part. The null-space of $(P\mathcal{X})$ is preserved. The same is not true for the pure boundary formulation, since multipole approximations are made on D, which alters the null-space of $(4\pi I + D)$.

A simple numerical experiment shows how accuracy is retained under multipole acceleration in the mixed finite-difference / boundary-element (FD/BE) formulation, but not in the pure boundary-element (BE) formulation. Consider two rectangular wires, both of dimensions 8:1:1, spaced 1 unit apart. At their near ends, one wire is connected to a step-voltage source, while the other is grounded. Simulated voltage waveforms at their far ends are shown in Figure 1. For the FD/BE method, the accelerated solution is indistinguishable from the explicit solution, while for the BE method, the accelerated results are clearly erroneous.

5 Application Experiments

Two fairly realistic three-dimensional interconnect examples are given here. The GMRES [3] iterative method is used for solving the linear systems in (6) and (13). It is assumed that all conductors are polysilicon, with $\rho = .02\ \Omega - cm$, and $\epsilon = 12$ both inside and outside the conductors, which imply $\tau = 2 \times 10^{-14} sec.$ All computations are performed on an IBM Model 590.

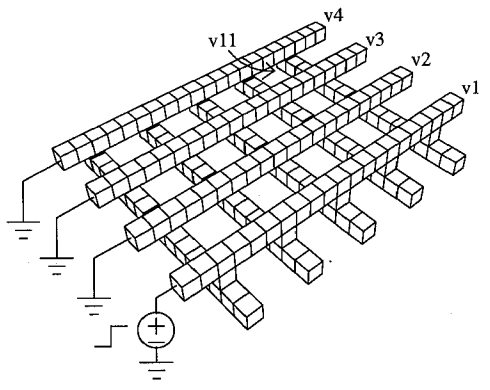

Figure 2: Clock driving five-conductor bus, with ground wires nearby.

Figure 2 displays a scenario in which a clock line connected to a step-voltage source is driving five parallel conductors in a bus configuration. Three nearby conductors, running parallel to the clock line, are grounded at one end but do not touch the bus. The conductor cross-sections all have dimensions $1\mu m \times 1\mu m$.

n	1	2	3	4	5
panels	684	2,736	6,156	10,944	17,100
FD time	–	0.3 %	3 %	7 %	11 %

Table 2: Problem size and FD time for clock/bus.

The waveforms computed using second-order multipole-FD/BE for various mesh refinements is shown in Figure 3. Table 2 lists the number of panels, or surface unknowns, used to discretize the problem. The parameter n denotes the number of sections per micron. The CPU time grows as N for the multipole-accelerated FD/BE method and as N^2 for both the explicit BE and the explicit FD/BE methods. This is shown is Figure 4. The same growth pattern is also observed in memory usage. For the $(n = 5)$ mesh, the multipole-FD/BE method is 15 times faster and requires nearly two orders of magnitude less memory than the explicit calculations.

The CPU time consumed by the interior finite-difference computation as a percentage of the total time grows with increasing mesh refinement but remains small, as shown in Table 2. This confirms the

earlier assertion that the boundary-element calculation is dominant.

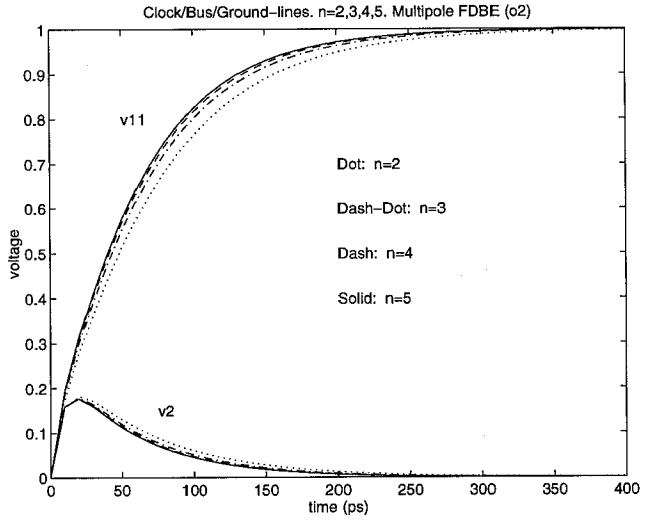

Figure 3: Multipole FD/BE solutions converge with mesh refinement.

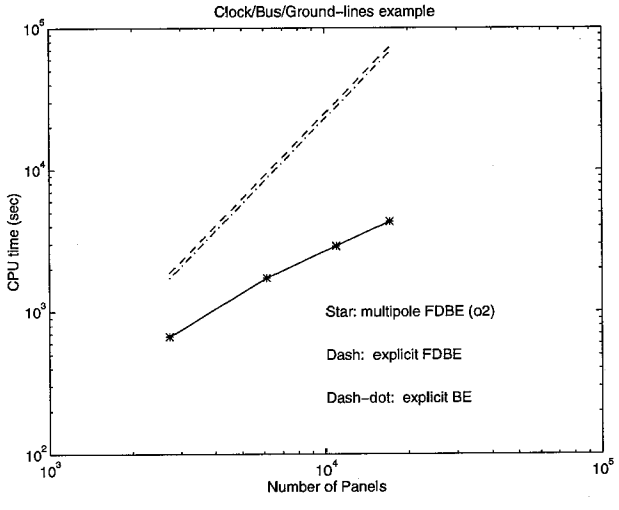

Figure 4: CPU time versus problem size.

n	1	2	3
panels	986	3,944	8,874
FD time	–	2 %	4 %

Table 3: Problem size and FD time for SRAM.

The second interconnect example, an SRAM cell, is shown in Figure 5. Table 3 lists the number of surface

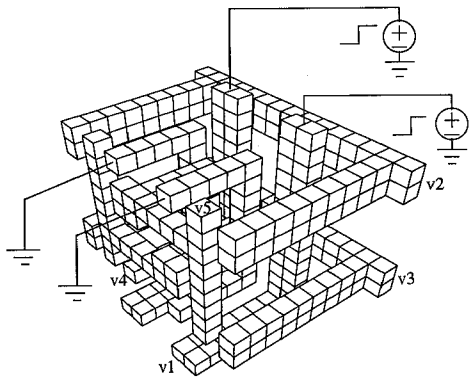

Figure 5: SRAM cell.

unknowns for three successive refinements, and Figure 6 shows the waveforms computed with explicit BE for $(n = 1)$ and with multipole-FD/BE for $(n = 2)$ and $(n = 3)$. It is seen that the coarse mesh $(n = 1)$ results in significant discretization errors, which necessitates using a finer discretization and thus the multipole-accelerated FDBE technique.

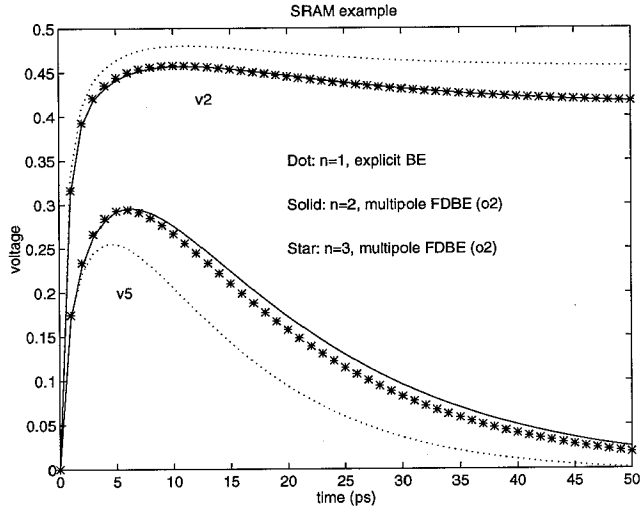

Figure 6: Waveforms computed using various mesh refinements.

6 Conclusions and Acknowledgements

In this paper, a mixed surface-volume technique is introduced for analyzing the three-dimensional transient interconnect problem. It is shown that the proposed method can be multipole-accelerated without

loss in accuracy, whereas a pure boundary formulation allows magnification of the multipole error by the condition number. The new approach reduces computational costs from $O(N^2)$ to $O(N)$.

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