# A Markov Chain Based Hierarchical Algorithm for Fabric-Aware Capacitance Extraction

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A Markov Chain Based Hierarchical Algorithm for Fabric-Aware Capacitance Extraction

Tarek El-Moselhy, Ibrahim (Abe) M. Elfadel, and Luca Daniel

Abstract—In this paper, we propose a hierarchical algorithm to compute the 3-D capacitances of a large number of topologically different layout configurations that are all assembled from the same basic layout motifs. Our algorithm uses the boundary element method in order to compute a Markov transition matrix (MTM) for each motif. The individual motifs are connected together by building a large Markov chain. Such Markov chain can be simulated extremely efficiently using Monte Carlo simulations (e.g., random walks). The main practical advantage of the proposed algorithm is its ability to extract the capacitance of a large number of layout configurations in a complexity that is basically independent of the number of configurations. For instance, in a large 3-D layout example, the capacitance calculation of 1000 different configurations assembled from the same motifs is accomplished in the time required to solve independently two configurations, i.e., a 500× speedup.

Index Terms—Integrated circuit interconnections, interconnected systems, large scale integration, Markov processes, Monte Carlo methods, parameter extraction, parasitic capacitance.

I. INTRODUCTION

RECENT integrated circuit technology nodes (32 nm and beyond) rely on regular patterns, uniform gridded designs and restricted design rules, in order to overcome many of the manufacturing-process related complications [1]–[3]. The main idea in such fabric-based design methodology, is to force designers to use a relatively small number of patterns (design fabrics, or design motifs), which are litho-friendly and preoptimized from a manufacturing prospective, in order to build arbitrary designs. As an example the reader is referred to Figs. 1 and 2, which represent two different configurations constructed from the same six motifs. Notice that with “configuration” we mean a structure constructed by a particular arrangement of the motifs. In this paper we propose a new hierarchical capacitance extraction algorithm specifically targeted to a large number of topologically-different structures which are constructed from a given set of motifs.

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Hierarchical algorithms rely on first subdividing the geometry into smaller subdomains, then resolving the local interactions by computing each subdomain independently and finally connecting the different subdomains together by resolving the global interactions. Fabric-based design methodologies do not require an initial “subdivision” operation but rather an “assembly” operation of predefined motifs. Nonetheless, hierarchical methods can still be the ideal choice to handle fabric-based designs, since each design motif can represent a subdomain. Unfortunately, in the majority of the standard hierarchical algorithms (e.g., [4]–[6]) resolving the global interactions constitutes the bottleneck of the computation, since it relies on assembling and solving a large linear system of equations. Such operation must be repeated for each configuration, hence standard hierarchical algorithms are not suitable for the efficient extraction of a large number of different configurations.

Recently, we have proposed a hierarchical technique [7] which efficiently resolves the global interaction by using Markov chain theory. In fact, in such algorithm resolving the global interactions is a lot less expensive than resolving the local interactions. The complexity of resolving the local
interactions is primarily related to the geometrical manipulations required by the standard floating random walk (FRW) algorithm. On the other hand, resolving the global interactions requires almost negligible complexity, since it involves only scalar computations as opposed to geometrical manipulations or large linear system solves.

Before proceeding with the details of this paper, we emphasize that just using “fast” or variation-aware extraction algorithms is not suitable for the task at hand. “Fast” algorithms (e.g., [8]–[11], etc.) rely on reducing the complexity of a single solve from $O(N^2)$ to $O(N)$. Unfortunately, in their present implementations, they do not reuse any of the computations between topologically-different configurations. Consequently, the complexity of such algorithms scales linearly with the total number of structures, which is computationally inefficient if such a number is large. Variation-aware extraction algorithms (e.g., [12]–[17]) typically handle problems, in which the topology is fixed, while the dimensions (width, thickness, or center–center distance) or shape (surface roughness) of the conductors vary. Hence, such methods do not account for variations which result in topological changes.

In this paper, the algorithm proposed in [7] is generalized. In particular, we demonstrate that the two steps corresponding to resolving the local and global interactions are totally independent (see Table I). Consequently, the particular technique best suited for computing each of the two steps can be independently chosen. For instance, it is well known that discretization based methods [such as boundary element method (BEM) or finite element method (FEM)] are significantly more efficient than discretization-free methods (such as FRW) for small/medium size structures. Consequently, in this paper we propose to use the BEM to compute the Markov transition matrices (MTMs) for each motif, unlike [7] in which the local interactions are resolved using the FRW. It is also known that for large systems, such as those that represent the global interactions, Monte Carlo based methods are significantly more efficient than linear system based methods. Consequently, we choose to resolve the global interactions by first building a large Markov chain from the computed MTMs. We then simulate the resulting Markov chain using random walks. The efficiency of the resulting algorithm is near-optimal for fabric-aware extraction. In other words, we can compute the capacitance of a large number of configurations, constructed from the same set of motifs, in a complexity that is practically independent of the number of configurations.

The rest of the paper is organized as follows. In Section II we develop our new hierarchical algorithm (BEM-MTM). In Section III we develop a fabric-aware BEM-MTM algorithm for 3-D capacitance extraction of a large number of configurations constructed by different recompositions of a set of motifs. Finally, in Section IV we show a variety of examples validating our algorithm.

## II. MAIN ALGORITHM: BEM-MTM

### A. Computing Local Interactions Within Motifs

In our hierarchical algorithm, the local interactions within each motif are captured by computing a Markov transition matrix (MTM) for each motif. Such a MTM represents the probability of moving from any point on the surface of the conductors inside the motif or any point on the boundary of the motif, to any point on the surface of conductors inside the motif or on the boundary of the motif. There are a variety of ways to define the MTM. In particular, in [7] the MTM is defined as the relation between the potential at the points on the surface of the conductors inside of the motif, or on the boundary of the motif and the potential at the same points. In this paper we define a more general MTM, which relates the charge at the points on the surface of the conductors inside of the motif or on the boundary of the motif to the potential at the same points. Such a MTM can therefore be interpreted as a capacitance matrix (see Fig. 3)

$$q_i = \sum_{j=1}^{N} C_{ij} v_j$$  \hfill (1)

where $q_i$ is the charge at point $i$, $v_j$ is the potential at point $j$ and $C_{ij}$ is the capacitance between $i$ and $j$. Notice that $v_j$ is the absolute potential relative to infinity. Equation (1) can be rewritten as

$$v_i C_{ii} - q_i = - \sum_{j=1 \& j \neq i}^{N} C_{ij} v_j.$$  \hfill (2)

Equation (2) can be written in matrix form

$$\text{diag}(C) \cdot v - q = -\Delta C \cdot v$$  \hfill (3)

where $\text{diag}(C)$ is a diagonal matrix whose diagonal elements are equal to those of $C$ and $\Delta C = C - \text{diag}(C)$.

**Lemma II.1:** The matrix $-(\text{diag}(C))^{-1} \Delta C$ is a MTM, in which the element $i, j$ represents the probability of moving from the node $i$ to the node $j$ inside of the same motif.

![Fig. 3. The capacitance matrix of a single motif describes the connectivity between the nodes.](image)
Proof: In order to prove that $-(\text{diag}\{C\})^{-1}\Delta C$ is a properly defined MTM we need to show that it satisfies the following three properties.

- The diagonal element of each row is equal to zero.
- All elements of each row are strictly nonnegative.
- The sum of any row is equal to 1.

The first statement is trivially true, since $\Delta C$ has zero diagonal elements. The second statement follows from the fact that the capacitance matrix has positive diagonal elements and negative off-diagonal elements [18]. The third statement follows from the fact that in any closed domain, where no field is allowed to escape, the sum of any row of the capacitance matrix is zero [18]. Consequently,

$$C_{ii} = -\sum_{j=1, j\neq i}^{N} C_{ij}.$$  
(4)

The sum of any row (e.g., the $i$th row) of $-(\text{diag}\{C\})^{-1}\Delta C$ is

$$\frac{1}{C_{ii}} \sum_{j=1, j\neq i}^{N} C_{ij}.$$  
(5)

Substituting (4) in (5)

$$\frac{1}{C_{ii}} \sum_{j=1, j\neq i}^{N} C_{ij} = 1.$$  
(6)

The motif MTM or equivalently the capacitance matrix in a closed domain (see Fig. 3) can be computed using any standard extraction algorithm, such as FRW, BEM, or FEM. In this paper, the MTM is computed using the BEM, since the motifs are typically small to medium size problems for which the BEM is very efficient. For ease of presentation, we assume that the medium is homogeneous with permittivity $\varepsilon$. For examples on how to apply the BEM in media with complex dielectric configurations, the reader is referred to [4], [5], [9]. Starting from the integral equation formulation

$$\frac{1}{2} \phi(r) = \int_{\Omega} \rho_{v}(r) G(r, r') d^{2}r' - \int_{\Gamma} \varepsilon \nabla_{n} G(r, r') \nabla_{n} \phi(r') d^{2}r'$$
$$+ \int_{\Gamma} \phi G(r, r') \nabla_{n} G(r, r') d^{2}r'$$  
(7)

where $\Omega$ is the computational domain, $\Gamma$ is the union of the boundary of the motif and the surfaces of the conductors, $\hat{n}$ is the unit normal vector to $\Gamma$, $\nabla_{n} = \hat{n} \cdot \nabla$, $G(r, r') = 1/4\pi \varepsilon \|r-r'\|$ is the free space Green’s function, $\rho_{v}(r)$ is the volumetric charge density, and $\phi(r)$ is the electric potential.

Using the fact that there are no volumetric charges $\rho_{v}(r) = 0$ and that the surface charge density $\rho_{s}(r') = -\varepsilon \nabla_{n} \phi(r')$, we obtain

$$\frac{1}{2} \phi(r) = \int_{\Gamma} G(r, r') j_{f}(r') d^{2}r'$$
$$+ \int_{\Gamma} \phi G(r, r') \nabla_{n} G(r, r') d^{2}r'.$$  
(8)

Equation (8) is solved for the unknown potential $\phi(r)$ and unknown surface charge density $\rho_{s}(r)$, which are defined every-where on $\Gamma$. For simplicity, both the charge density and the potential are discretized using piecewise constant basis functions supported on rectangular panels. Then, collocation testing is used in order to obtain a linear systems of equations of the form

$$\left(\frac{1}{2} I - M_{n}\right) \mathbf{v} = \mathbf{Mq}$$  
(9)

where $\mathbf{v}$ is a vector of the potential coefficients and $\mathbf{q}$ is a vector of the charge coefficients (notice the use of charges not charge densities), and

$$M_{n}(i, j) = \int_{S_{j}} \frac{\varepsilon_{n} G(r_{i}, r') d^{2}r'}{\alpha_{i}}$$  
(10)

$$M(i, j) = \int_{S_{j}} \frac{G(r_{i}, r') d^{2}r'}{\alpha_{i}}$$  
(11)

where $\varepsilon_{n}$ refers to the principal value of the integral and $\alpha_{i}$ refers to the area of panel $i$. Notice that both integrals are available in analytical closed form. Using (9) we obtain

$$\mathbf{q} = M^{-1} \left(\frac{1}{2} I - M_{n}\right) \mathbf{v}$$  
(12)

which leads to the following motif MTM

$$C = M^{-1} \left(\frac{1}{2} I - M_{n}\right).$$  
(13)

B. Resolving the Global Interactions

When motifs are connected together, two different boundary conditions must be satisfied, namely, the continuity of the potential, and the continuity of the displacement field. Notice that there is no charge accumulation at the interface between motifs. When connecting motifs, each discretization panel can belong to at most two motifs. Writing (2) at two neighboring motifs (see Fig. 4), and summing the resulting expressions we obtain

$$\mathbf{v}_{i}^{(1)} C_{ii}^{(1)} + \mathbf{q}_{i}^{(1)} + \mathbf{v}_{i}^{(2)} C_{ii}^{(2)} + \mathbf{q}_{i}^{(2)}$$
$$= - \sum_{j=1, j\neq i}^{N} C_{ij}^{(1)} \mathbf{v}_{j}^{(1)} - \sum_{j=1, j\neq i}^{N} C_{ij}^{(2)} \mathbf{v}_{j}^{(2)}$$  
(14)

where the superscripts (1) and (2) refer to local quantities of the first motif and of the second motif, respectively. We have assumed without loss of generality that the common interface point is given the local index $j$ in both neighboring motifs. Consequently, at the boundary point $i$: $\mathbf{v}_{i}^{(1)} = \mathbf{v}_{i}^{(2)} = \mathbf{v}_{i}^{(g)}$ and $\mathbf{q}_{i}^{(1)} = \mathbf{q}_{i}^{(2)} = 0$ we obtain

$$\mathbf{v}_{i}^{(g)} \left( C_{ii}^{(1)} + C_{ii}^{(2)} \right) = - \sum_{j=1, j\neq i}^{N} C_{ij}^{(1)} \mathbf{v}_{j}^{(1)} - \sum_{j=1, j\neq i}^{N} C_{ij}^{(2)} \mathbf{v}_{j}^{(2)}$$  
(15)

which leads to

$$\mathbf{v}_{i}^{(g)} = \sum_{j=1, j\neq i}^{N} \left( C_{ij}^{(1)} + C_{ij}^{(2)} \right) \mathbf{v}_{j}^{(1)} + \sum_{j=1, j\neq i}^{N} \left( C_{ij}^{(1)} + C_{ij}^{(2)} \right) \mathbf{v}_{j}^{(2)}.$$  
(16)
where the summation is over all the panels discretizing the surface of conductor $I$. Consequently, the objective is to compute each individual $q_i$, which is achieved by resorting to (2). Furthermore, since in any standard mutual capacitance extraction setup the voltage at the target wire is set to 0, i.e., $v_i = 0$, (2) is reduced to

$$q_i = \left( -C_{ii} \right) \sum_{j=1, j \neq i}^N \frac{-C_{ij}v_j}{C_{ii}}. \quad (19)$$

Notice that the term $-C_{ij}/C_{ii}$ represents the probability of making a transition from the starting panel $i$ to some other panel $j$ inside or on the boundary of the same motif. Consequently, the summation is computed using random walk methods by choosing a point on the motif boundary or on a conductor surface based on the probabilities $-C_{ij}/C_{ii}$. If the chosen point is on a panel with prescribed potential $v_j$, then the path is assigned the random variable $-C_{ij}v_j$ and is terminated. Otherwise, the chosen point is on the boundary of the motif, and the path needs to be completed until reaching a conductor anywhere in the configuration. To complete the path, equation (17) is similarly computed using random walks. In such computation the weighting functions $u_{ij} = -C_{ij}/C_{ii}$ are interpreted as the probability of making a transition from the point $i$ to the point $j$ in the global network. This is implemented by drawing randomly a number $r$ from a uniform distribution between 0 and 1. The point $j$ is chosen such that $\sum_{k=1}^{i-1} w_{ik} < r$ and $\sum_{k=1}^{i} w_{ik} > r$. If point $j$ is on a conductor surface then the random variable $-C_{ij}v_j$ [see (19)] is assigned to the path and the path is terminated. The process of generating paths is then repeated a large number of times. The unknown charge $q_i$ is finally computed using $q_i = -C_{ii}E[v_j]$, where $E[]$ is the expectation operator

$$q_i = -C_{ii}\frac{\# \text{ of paths from } i \text{ to } j}{\text{total } \# \text{ of paths starting from } i}. \quad (20)$$

**Important Note:** Since in the capacitance extraction setup only one conductor is assigned a nonzero potential at a time, only paths terminating at that particular conductor will have a nonzero contribution to the random variables. Consequently, the capacitance from conductor $I$ to all other conductors can be computed simultaneously. If the target conductor is the same as the source conductor (i.e., we want to extract the self capacitance of a conductor) then $v_i$ in (2) is equal to 1 and the value of $C_{ii}$ is added to $q_i$.

Algorithm 1 summarizes our complete algorithm for computing the $I$th row of the capacitance matrix. Fig. 5 shows two different possible paths.

### D. Theoretical Analysis of BEM-MTM

Many standard “absorbing Markov chain” theorems and well known results can be exploited to certify properties of our BEM-MTM algorithm once we show how it is possible to appropriately construct a large MTM $T$ for the entire configuration

$$T = \begin{bmatrix} Q & R \\ 0 & I \end{bmatrix} \quad (21)$$
Algorithm 1 BEM-MTM for a given configuration

1: repeat
2: choose randomly a point \( i \) on the the surface of the target conductor \( I \).
3: using (19) take a step starting from point \( i \)
4: if reached a point on the interface between motifs then
5: repeat
6: make a transition using the capacitance matrices of both motifs defining the interface (see (17))
7: until a conductor or a configuration boundary are reached
8: end if
9: if terminated on a conductor \( J \) then
10: add \(-C_{ij}\) to capacitance \( C(I,J)\)
11: else \{ terminated on configuration boundary \}
12: add \(-C_{ij}\) to stray capacitance \( C(I,0)\)
13: end if
14: \( C(I,J)\) \(\leftarrow\) \( C(I,J) + C_{ij} \)
15: until convergence achieved
16: divide \( C(I,:)\) by the total number of walks

**Fig. 5.** Two paths starting from point \( i \). The first terminates in one step on conductor \( I \), the second terminates in three steps on conductor \( J \) in a different motif.

where \( Q \) is the transition probability matrix between “transient states” (in our case any point on the interface between motifs as shown in Fig. 6); \( R \) is the transition probability matrix from the transient states to the “absorbing states” (in our case all the conductors and any point on the external configuration boundary). Matrices \( 0 \) and \( I \) simply define the behavior of the absorbing states: once an absorbing state is reached the probability to remain in it is one, and consequently the probability to transition to any other state is zero. The upper part \([Q\ R]\) of the MTM \( T\) can be related to the individual MTMs of each motif using the Law of Total Probability

\[
\begin{bmatrix}
Q & R
\end{bmatrix} (i,j) = \frac{C_{ij}}{C_{ii}} (22)
\]

where \( C_{ij} \) is the total capacitance between the points \( i \) and \( j \) in the global capacitance network; and \( C_{ii} \) is the total capacitance connected to node \( i \). Notice that there is no capacitance between \( j \) and \( j \) if they do not belong to the same motif, there is a single capacitance if they belong to the same motif but not the same interface, and there are two different capacitances if \( i \) and \( j \) belong to a common interface.

Having cast our BEM-MTM algorithm as an absorbing Markov chain problem it is easy to rigorously answer many legitimate questions using the literature available on that topic [23]. For instance, the following theorem can be used to prove the termination of each BEM-MTM “path” in a finite number of transitions, and to even provide a precise estimate on the average number of transitions before termination.

**Theorem II.1:** Assume that BEM-MTM starts at a point \( i \) on an interface between motifs (i.e., a transient state), then the average length of the walk on interfaces, or expected number of transitions before reaching a conductor or the configuration boundary (i.e., an absorbing state), is finite and is given by the row sum of the \( i \)th row in the “fundamental matrix” \( N = (I \ - \ Q)^{-1} \)

**Proof:** The proof follows directly from Theorem 3.3.5 in [23].

**E. Computational Complexity**

**Time:** Assume that the structure was assembled using \( N_{M} \) different kind of motifs and that each motif \( k \) is discretized using a total of \( n_{k} \) panels (on boundary and conductor surfaces). The complexity of computing the \( k \)th motif MTMs is \( O(n_{k}^{2}) \). Notice that the inverted matrix is exactly the capacitance matrix of the first type Fredholm formulation, which means that we can use fast algorithms to compute \( n_{k} \) matrix solves. However, in general the independent motifs are sufficiently require fast algorithms. All the motifs are independent. Consequently, the computation is embarrassingly parallelizable and the total complexity for computing all motifs is bounded by \( \sum_{k}^{N_{M}} O(n_{k}^{2}/N_{PROC}) \), where \( N_{PROC} \) is the total number of processors.

The second part of the algorithm consists of resolving the global interaction. For that we need to initiate a large number of random walks. The complexity is linear in the number of walks \( O(N_{w}) \). This part of the algorithm is also embarrassingly parallelizable, consequently the complexity is \( O(N_{w}/N_{PROC}) \). The main computational advantage of our algorithm is that the complexity constant associated with this part of the computation
is very small, since there are absolutely no geometrical manipulations involved. Instead, all transitions, are implemented by purely numeric manipulations, and are consequently extremely cheap.

**Memory:** The memory required for resolving the local interactions is \( O(\text{max} \cdot \text{size}^2) \), which is the memory required for the computation of the MTM of the motif discretized using the largest number of panels [see (9)]. On the other hand, resolving the global interactions requires storing the MTMs of all motifs for a total memory of only \( O(\sum_{k}^{NM} \text{size}_k) \), since in general the MTMs are very sparse (an example will be presented in the result section). Typically, a total of 100 transition matrices, corresponding to 100 different kind of motifs, can be stored in 2 GB of RAM. Notice that the actual number of instantiations of such motifs in the design configurations can be orders of magnitude larger than the number of kinds of motifs without any significant increase of the memory requirement.

**F. Comparison Versus Other Hierarchical Algorithms**

Compared to the HFRW [7] (which is a FRM-MTM algorithm), our new algorithm avoids using the computationally expensive FRW to compute the MTM of each motif. Such computations are expensive since they involve geometrical manipulations. As mentioned previously, our algorithm does not involve any of the FRW geometrical manipulations. Similar to the HFRW algorithm, our BEM-MTM uses the MTMs to resolve the global interactions. On the other hand, the main advantage of using the HFRW is that it can handle edge-defined variations extremely efficiently, whereas the BEM-MTM can only handle topological variations.

The main difference between our algorithm and the standard BEM hierarchical methods ([4], [5]) is that our algorithm resolves the global interactions without assembling/solving any expensive linear systems. Instead, our algorithm resolves the global interactions using random walks to simulate the Markov Chains. For large structures, such random walk methods are significantly more efficient than solving large linear systems of equations. In addition, BEM-MTM fully exploits the local nature of the capacitance extraction problem. Moreover, the BEM-MTM can efficiently extract the capacitance of a very large number of topologically different configurations constructed from the same set of motifs (see Section III).

Compared to approximate hierarchical algorithms [6], [11] and window based techniques [24], [25], which all rely on some form of approximation to achieve computational efficiency, our BEM-MTM algorithm is exact. In general, one of the main advantages of our BEM-MTM is that it exploits the local nature of the capacitance problem to achieve computational efficiency without the need to introduce approximations. In particular, the random walk simulation of the Markov chain exploits the fact that most of the capacitance of a wire is determined by the nearby interactions, since paths connecting a conductor to its immediate neighbors are typically very short and are computed extremely efficiently.

**G. Comparison Versus the Standard FRW**

There is apparent similarity between the proposed algorithm and the standard FRW [26], since the latter relies on first determining a transition domain, then making a transition from inside of the transition domain to its boundary, and repeating such process until the path terminates at a conductor surface with known potential. However, there exist a variety of fundamental differences between the two algorithms. Foremost, in the FRW the notion of transition domains is restricted. Indeed, in the standard FRW [26] a transition domain is a domain that includes no conductors and must have homogeneous media. In the generalized FRW [16] the transition domains are allowed to include nonhomogeneous media, however, they are not allowed to include any charged conductors. Such constraints typically result in small transition domains. On the other hand, in the BEM-MTM the notion of transition domain is generalized to be basically any closed domain. Indeed, by this new definition, the transition domain is now allowed to include complex dielectric structures, floating potential metal fills and even charged conductors. Such generality allows for declaring a whole predefined motif as a single transition domain.

Another difference is that due to the large constrains on what is defined as a transition domain in the FRW, the transition probability matrix is available in closed form and does not need to be numerically computed. Even in the generalized FRW, since the domain is relatively constrained and small in size, computing the transition matrix numerically is a trivial task. In our algorithm since the transition domains are large and general, the MTMs must be computed numerically. However, since the domains are predetermined by the set of motifs available in the fabric-aware design methodology, the MTMs can be precomputed only once for a given technology and then reused for all walks in all design configurations that use those motifs.

The most important difference is that in the FRW the transition domains are overlapping and are constructed online along the way of the path. Most of the computational time is spent on the geometrical manipulations required to determine the dimensions of the transition domains. In the BEM-MTM algorithm, the transition domains (which actually coincide with the design motifs) are non-overlapping, and are predetermined (rather than recomputed at each step). Therefore, the BEM-MTM algorithm does not require any geometrical manipulations. Indeed, in the BEM-MTM the walk, which starts and terminates at conductor surfaces and proceeds only on interfaces between motifs, is fully implemented using only numerical manipulations without the need for determining any transition domain or any other geometrical manipulations.

To summarize, our algorithm could be interpreted as an extremely generalized FRW in which the domains are predetermined, nonoverlapping, and large. The transition probability matrix is computed once by using a discretization-based solution to a given PDE. In terms of implementation, all FRW-related geometrical manipulations are removed and only the underlying Markov chain is very efficiently simulated using random walks.

**III. Fabric-Aware Extraction**

The most important advantage, and in general the main motivation behind using the BEM-MTM algorithm, is that it offers a very efficient algorithm to extract the capacitance of a very
Algorithm 2 BEM-MTM for all configurations

1:  for each motif kind do
2:      compute the MTM
3:  end for
4:  for each desired capacitance matrix row $C(I,:)$ do
5:      repeat
6:          Make a random walk step starting from conductor $I$
7:          if step reached a point on the interface between motifs then
8:              for each configuration do
9:                  use MTMs to walk on interfaces and terminate
10:                 on a conductor or configuration boundary
11:                 add $-C_{d}$ to appropriate capacitance
12:              end for
13:          else {step reached a conductor}
14:              add $-C_{d}$ to appropriate capacitance
15:      end if
16:      $C(I,I) \leftarrow C(I,I) + C_{d}$
17:  until convergence achieved
18:  divide $C(I,:)$ by the total number of walks

large number of configurations constructed by different arrangements of a given set of motifs. Indeed, since in our BEM-MTM resolving the global interaction is cheaper than computing the local interactions, we can afford to repeat such a computation for a very large number of different configurations without significantly increasing the complexity of our algorithm. Furthermore, the majority of paths (corresponding to the self term and the strong coupling terms) terminate in the motif containing the target conductor and do not even have to be continued. Consequently, such paths are computed only once and are shared among all different configurations without the need for any recomputations. This in turn explains our observation that the BEM-MTM exploits the local nature of the capacitance extraction problem.

Algorithm 2 summarizes the steps of our proposed approach for 3-D capacitance extraction of a large number of configurations constructed by different recompositions of a set of motifs. Recall that if we have $N_{M}$ motif instantiations then there are $O(N_{M}!)$ possible different configurations.

Since all configurations are constructed from the same set of $N_{M} \ll N_{T}$ motifs, the $N_{M}$ motif MTMs can be precomputed separately as shown in Step 2. The complexity of this part of the algorithm depends linearly on the number of different kinds of motifs $O(N_{M})$, and does not depend on the total number of configurations, $O(N_{T}!)$. Step 6 in Algorithm 2 is independent of the configuration structure, and therefore it is implemented once per motif and reused for all configurations. This step is very efficient since it involves only generating one random variable and choosing a corresponding point on the domain boundary or a conductor surface.

The remaining part of each path depends on the particular recomposition of the motifs, therefore it must be executed separately for each configuration. Since this part of the algorithm does not involve any geometrical manipulations it is extremely cheap. Consequently, the bottleneck of the algorithm is Step 2, and the complexity of our algorithm is almost completely independent of the total number of configurations.

IV. RESULTS

Unless otherwise stated the reported results are obtained using our own Matlab implementations of the corresponding algorithms on a Intel Duo CPU at 2.4 GHz with 2 GB of memory. Unless otherwise stated, all floating random walk related results have been obtained by using a total of one million random walks, i.e., $N_{rw} = 10^6$.

A. Accuracy Validation

The first example validates the accuracy of the proposed algorithm. A cross section of the 3-D geometry for this example is shown in Fig. 7, and is composed of 12 conductors. The geometry was assembled using four different motifs. In addition, empty motifs are added at the boundary (shown only partially in Fig. 7) to mimic the infinity boundary condition. In order to verify the accuracy of our approach, we extracted the capacitance between a target conductor in motif 1 (see Fig. 7) and all the other 11 conductors using both our BEM-MTM and the standard BEM method. Using $2 \times 10^5$ paths, the BEM-MTM is 10 times slower than the standard BEM and obtained for all extracted capacitances a 0.1% accuracy compared to the BEM method.

B. A Small 3-D Fabric-Aware Extraction Example

In this example we use the same motifs used in Fig. 7 (from the previous example IV-A) to construct a total of $4! = 24$ different configurations, corresponding to all possible different recompositions of the four internal motifs. The capacitance matrices of each of the configurations are computed using both our BEM-MTM and the standard BEM. All the values of the computed capacitances for each configuration are within 0.5% of the values computed using the standard BEM. The total time to compute the capacitance matrices of all 24 configurations using our BEM-MTM is about $(12 \times)$ the time required to compute the capacitance matrix of just one configuration using the standard
BEM. This corresponds to a $2 \times$ speedup. The reason we did not obtain large speed-up ratios is that this example is small.

C. A Large 3-D Example

In this subsection we demonstrate that the BEM-MTM can treat large 3-D structures very efficiently. The example under consideration is a five layer structure (Fig. 8). Two of such layers contain 100 cubic shaped conductors arranged on a $10 \times 10$ grid. The size of the conductors is 100 nm. These small conductors represent “metal fill,” i.e., small floating potential conductors inserted in empty regions of the layout to facilitate the planarization. Each of the other three layers contain 3 parallel long wires of dimensions $100 \ \text{nm} \times 1400 \ \text{nm} \times 100 \ \text{nm}$. The wires are separated by 100 nm. Each of the five layers is 300 nm thick and has a unique dielectric constant. Each layer is treated as a motif. We recompose such motifs to construct a total of 120 different configurations. Notice that every configuration includes a total of 209 total conductors. Four different capacitances are extracted from each configuration.

The time required to compute the MTMs of the five motifs is approximately 6 min. The largest MTM is of dimensions $1536 \times 1636$, and is 95% sparse (Fig. 9). The computational time required to solve all possible 120 configurations is 15 min. Using the HFRW [7] to compute the capacitance of all 120 configurations requires 30 min. Running a standard boundary element method hierarchical algorithm (HBBEM) on all 120 configurations requires about 600 min. Running the standard FRW on the same example would require an estimated 1800 min. Running FastCap (C code) on the same set of 120 configurations with the same 5% accuracy requires a total of 270 min. Hence, our Matlab BEM-MTM is $1.5 \times$ faster than HFRW, $20 \times$ faster than Matlab HBBEM, $9 \times$ faster than C-code FastCap and $60 \times$ faster than the standard FRW.

D. A Very Large Example

In this example we extract the capacitances of a 3-D, 10-layer very large structure. Each layer is composed of 20 parallel long conductors and has a unique dielectric constant. Each layer was assembled using 4 motifs, resulting in a total of 40 motifs. On average, each motif is discretized using 4000 unknowns. The time used to compute the complete capacitance matrix for all motifs is less than 50 min. The average transition matrix is about 99% sparse, which means that storing all the transition matrices requires less 0.2 GB of memory. Fig. 10 shows the sparsity pattern corresponding to the MTM of the largest domain. Using the computed MTMs we extract the capacitance of a total of 1000 randomly generated different configurations in 45 min, which corresponds to slightly less than the time required to compute the MTMs. When using the HFRW [7] to compute the capacitance of all 1000 configurations 495 min are required (450 min to compute the MTMs and 45 min to extract the capacitance of the configurations). Hence, our algorithm provides $5 \times$ reduction in computational time. Due to large memory requirements (more than 4 GB), this example cannot be solved using our implementation of the standard hierarchical algorithms [4], [5] (which rely on assembling/solving a linear systems of equations).

\[^{1}\text{Notice that the HFRW requires 15 min to compute the different MTMs and 15 min to do the subsequent extraction. Our BEM-MTM provides only 2.5x reduction in computational times required to compute the MTMs, since the motifs in this example are very dense and can therefore be efficiently computed using the FRW.}\]
V. CONCLUSION

In this paper, we have presented a hierarchical extraction algorithm for computing the 3-D capacitances of a large number of layout configurations that, although topologically different, are all assembled from the same layout motifs. Our BEM-MTM algorithm uses the boundary element method to efficiently compute a MTM for each motif. The motifs are connected together to form a large Markov chain. Such a chain is then simulated very efficiently using random walks. Consequently, our algorithm avoids the main complexity of standard hierarchical algorithms by not relying on assembling/solving linear systems to resolve the global interactions. Furthermore, our approach does not rely on approximations and trade-off between accuracy and computational efficiency. The main advantage of our algorithm is its extreme efficiency in extracting the capacitance matrix of a large number of configurations constructed by different recompositions of the same set of motifs. We have observed that its complexity is almost independent of the number of configurations. In particular, in a large example, the total time required to compute all the capacitance matrices of 1000 different 3-D configurations is only two times the time required for solving a single configuration. This is equivalent to a 500× speedup.

REFERENCES


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