The Hierarchical h-Adaptive 3-D Boundary Element Computation of VLSI Interconnect Capacitance*

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Abstract: In VLSI circuits with deep sub-micron, the parasitic capacitance from interconnect is a very important factor determining circuit performances such as power and time-delay. The Boundary Element Method(BEM) is an effective tool for solving Laplacian's equation applied in the parasitic capacitance extraction. In this paper, a hierarchical h-adaptive BEM is presented . It constructs a 3-D linear hierarchical shape function based on constant boundary element and uses previous computations and solutions. Hence, it reduces much computation in adaptive procedure. Besides, a combination of residual-type estimator and reduced Z-Z error estimator for more reliable and efficient estimation of error is presented. Some numerical results show that this method is effective.

Key words: Parasitic Capacitance, Boundary Element Method, Hierarchical h-Adaptive Computation, VLSI

1 Introduction

In deep-submicron VLSI circuits, with the feature sizes scaled down and device density increased, the parasitic capacitance of interconnecting conductors is becoming dominant in governing circuit delay and power consuming[5,13]. To compute the capacitance , the Laplacian's equation can be solved numerically over the simulated region with the specified boundary conditions.

A variety of numerical methods known as the finite difference method (FDM), finite element method (FEM) and boundary element method (BEM) can be used for solving the Laplacian's equation characterizing the parasitic capacitance. Recently, the BEM[2,3,5,13] is commonly used as a competitive tool with the advantages of high accuracy, less degree of freedom and strong ability to handle complex boundary geometry. Both partitioning of elements and degree of interpolation polynomials approximating the variables in the boundary elements are the key factors which affect computational accuracy of the BEM. Now, a 3-D interconnecting parasitic capacitor from the practical layout often is a very complicated structure involving 5~6 layers of different dielectrics and many pieces of conductors up to several hundreds. It is very difficult to achieve a rational and scientific discretization by a manual process. So, it is necessary to get help from the mathematics like adaptive computation for higher computational accuracy and efficiency. Several efficient adaptive schemes classified as h-, p-, and hp-refinement were proposed for improving the accuracy of boundary element computation[6]. The h-adaptive version[7,14] means that improvement of the global accuracy can be achieved by locally refining mesh without change of the interpolation degree. The p-adaptive version[15] means that the global computation accuracy can be improved by locally refining the degree of the interpolation polynomial without changing partitioning of the boundary elements. The hp-adaptive version[16] is a combination of the above two adaptive schemes. In this paper, the h-adaptive scheme is used because of its good stability from using lower degree of interpolation polynomials.

As adaptive approaches are iterative procedures, in which the global matrix must be formed at each refinement step because of introducing additional refinements in some elements, its computational cost becomes high. To overcome this difficulty, it is natural that the higher interpolations are obtained under maintaining the previous interpolation basis functions used. Thus a hierarchical definition of the interpolation basis functions is crucial for efficiency of the adaptive methods. The hierarchical adaptive computations can be understood as those in a Fourier series expansion new terms are introduced in the manner of maintaining the previous terms unaltered[8,15]. In the boundary element context, articles [9] and [14] proposed some methods of constructing linear, quadratic and quartic h-hierarchical shape functions in two-dimensional(2-D) cases. Based on these works, we got improvements in two aspects . First, h-hierarchical shape functions in 3-D boundary element analysis , which are the extension of those in 2-D case, are formed . Second , the linear hierarchical shape functions are based on constant element , not linear element , thus it avoids much difficulty in dealing with discontinuity of the normal electrical field at corner points. Furthermore, we proposed a reduced Zienkiewicz-Zhu(Z-Z) error estimator[12] , which makes the error estimation more efficient.

2 The boundary element computation of capacitance

Generally, the interconnecting capacitor from the VLSI circuits can be treated as a 3-D structure, which is characterized by the Laplacian's equation with mixed boundary conditions, including many conductors embedded in an arbitrary piecewise constant dielectric medium[5,13]. For simplicity, the Laplacian's equation with mixed boundary condition in a medium is shown as follows.

$$\begin{cases} \nabla^2 u = 0 & \text{in region } \Omega \\ u = u_0 & \text{on Dirichlet boundary } \Gamma_u \\ q = \dfrac{\partial u}{\partial \mathbf{n}} = 0 & \text{on Neumann boundary } \Gamma_q, \end{cases} \qquad (1)$$

where the electrical potential u is a function of (x,y,z), **n** is the outward unit normal. Using the Green formula and property of the fundamental solution u* of the Laplacian's equation, the partial differential equation (1) can be transformed to a set of the direct boundary integral

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equations[1,2,4]:

$$c_i u_i = \int_\Gamma q^* u d\Gamma - \int_\Gamma u^* q d\Gamma \qquad (2)$$

where $q^* = \dfrac{\partial u^*}{\partial \mathbf{n}}$, $\Gamma = \Gamma_u + \Gamma_q$ is boundary of the region Ω, and c_i is a constant dependent on geometry of the boundary Γ in neighborhood at the source point i. Then the boundary Γ needs to be discretized and equation (2) is numerically solved by the BEM[1,2].

Since discretization made by inexperienced users is a tedious work and often results in large computation error , we should develop an adaptive mesh refinement scheme to insure the accuracy of solution.

3 Hierarchical shape functions in h-adaptive refinement

As most of the interconnecting conductors are cuboid, we use quadrilateral elements (rectangular elements as many as possible, particularly) as the initial mesh in the adaptive process for smaller discretization error[17] and its easy implementation. It was supposed that the initial mesh needs to be locally refined and the h-hierarchical shape functions need to be added on those subdivided elements. The key point of constructing the h-hierarchical shape functions is that the hierarchical functions only add new terms on the new subdivided elements , maintaining the old term on the initial mesh unchanged[8,9] . Note that the new added terms must be linear independent with the existing terms. Next we will show how to build the hierarchical functions on a rectangle element .

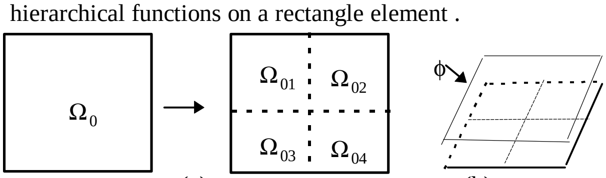


Fig. 1 (a) A rectangle element Ω_0 needs to be subdivided into four sub-elements $\Omega_{01} \sim \Omega_{04}$, (b) the constant shape function φ_0 on Ω_0.

In figure 1, Ω_0 is a rectangle element with its constant shape function $\varphi_0 = 1$ shown in (b). If Ω_0 is subdivided into four sub-elements and on each sub-element the shape function is also constant, i.e., $\phi_{01} = \phi_{02} = \phi_{03} = \phi_{04} = 1$, immediately , it can be seen that the new added functions $\phi_{01} \sim \varphi_{04}$ are linearly dependent on the initial shape function ϕ_0. Obviously, it leads to singularity of the linear equation system from discretizing the integral equation (2). So this kind of constant shape functions is not valid in the hierarchical computations.

In this paper , we proposed a linear hierarchical shape functions based on constant elements. The shape function of the initial element is kept constant , but the new added shape functions are the pyramid-like linear functions defined on every sub-element. For example, in region Ω_{01}, the shape function φ_{01} is set 1 at the center O of Ω_{01} and 0 on the four edges of the region. This is shown in Fig. 2. Below, we show how to generate the shape function j_{01} on Ω_{01}.

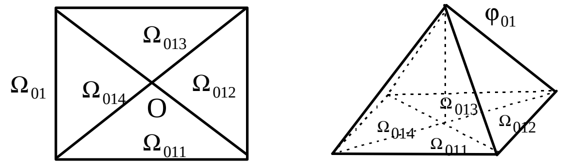


Fig. 2 Pyramid-like shape function φ_{01} on region Ω_{01}.

Denoting triangular area Ω_{011} by △OAB, it can be transformed into a regular isoparametric triangular element by using the local area coordinate ξ, η, as shown in Fig. 3.

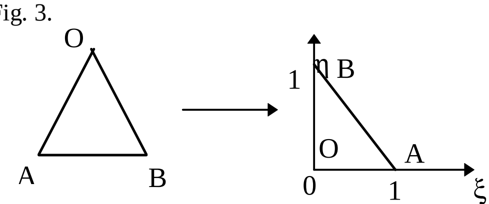


Fig. 3 Transformation of isoparametric triangular element.

In subregion Ω_{011} of Ω_{01}, using local area coordinate, the hierarchical linear function ϕ_{011}, which is a part of the shape function j_{01} defined above, can be written as follows:

$$\phi_{011} = 1 - \xi - \eta \qquad (3)$$

Also, the hierarchical functions ϕ_{012}、ϕ_{013} and ϕ_{014} on subregions Ω_{012}、Ω_{013} and Ω_{014} are similarly got. Let us call the constant shape function φ_0 the 0th level shape function of the h-hierarchical shape functions on the element Ω_0. The shape function ϕ_{01} constituted by $\varphi_{011} \sim \phi_{014}$ defined on subregions $\Omega_{011} \sim \Omega_{014}$ of Ω_{01} together with the shape functions $\phi_{02} \sim \varphi_{04}$ on subregions Ω_{02}、Ω_{03} and Ω_{04} composes the 1st level shape function on the element Ω_0. Apparently, the 1st level functions $\phi_{01} \sim \varphi_{04}$ are linearly independent on the 0th shape function ϕ_0. Based on this kind of hierarchical functions, if any sub-element of the element Ω_0 needs to be further refined, the pyramid-like shape functions with higher level can be formed, similarly.

In the h-adaptive BEM, the main advantage of using hierarchical shape functions is utilizing previous computation and part of solutions when locally refining the mesh. This fact can be explained in detail. Suppose that the coefficient matrix $A_{(n)}$ of the discrete linear system is corresponding to a mesh $M_{(n)}$ with n d.o.f. (degree of freedom) and it can be written as follows:

$$A_{(n)} x^{(n)} = b^{(n)} \qquad (4)$$

When the mesh $M_{(n)}$ is locally refined to a new mesh $M_{(n+m)}$ with m new d.o.f. introduced, the system of linear equations formed by using the hierarchical shape functions will have following form:

$$\begin{bmatrix} A_{(n)} & A_{(n,m)} \\ A_{(m,n)} & A_{(m)} \end{bmatrix} \begin{bmatrix} x^{(n)} \\ x^{(m)} \end{bmatrix} = \begin{bmatrix} b^{(n)} \\ b^{(m)} \end{bmatrix} \qquad (5)$$

where $A_{(n)}$ in the equation (4) is presented as a part of the coefficient matrix of the equation (5) because of preserving all of the previous shape functions in forming the refined equation (5).

In contrast, if using the shape functions without the hierarchy, the refined linear system corresponding to the new $M_{(n+m)}$ with (n+m) d.o.f. should be formed as follows:

$$A_{(n+m)}x^{(n+m)} = b^{(n+m)} \tag{6}$$

where all items of the coefficient matrix $A_{(n+m)}$ need to be calculated again[8]. So, using the hierarchical shape functions can greatly save the computational consumption in the h-adaptive boundary element analysis.

4 Error estimation and adaptive tactics

The adaptive procedure requires reliable and efficient method to estimate the discretization errors . Generally, there are two different methods of posteriori error estimation for boundary element methods : residual-type estimator[10,11,14] and non-residual-type estimator[12]. In this paper, a combination of them is presented to give a reliable and efficient error estimator.

After equation (2) is solved , both approximate potential $\bar{u}$ and normal field $\bar{q}$ on the boundary Γ are got. With reference to the equation (2), residual is defined as:

$$r_i = c_i u_i + \int_\Gamma q^* \bar{u} d\Gamma - \int_\Gamma u^* \bar{q} d\Gamma \tag{7}$$

where r_i is the residual at point i[11]. If $\bar{u}$ and $\bar{q}$ are exact to u and q anywhere, r_i will be zero at any point i. So, we can use r_i to indicate the discretization error at point i . Note that at every collocation point the residual r_i is equal to zero. For each boundary element Γ_j the local error estimator can be defined as:

$$\eta_j = \|r\|_{L2} = \sqrt{\int_{\Gamma_j} r^2 d\Gamma} \tag{8}$$

to indicate whether the element Γ_j should be refined.

At the same time, the global error estimator of k[th] refinement can be defined as follows:

$$\eta^k = \left(\sum_{j=1}^{N} \eta_j\right) / N \tag{9}$$

where N is number of all boundary elements. For a given accuracy e , the global error estimator η^k may be used to judge whether the adaptive computation should be stopped.

Computation complexity of the above residual-type estimator is $O(N^2)$. It requires much computation cost when N is large. In our algorithm, the initial mesh is set coarse enough that it can just describe the geometry of the bodies and boundary condition. This makes the computation cost of estimator not very large. After the initial mesh is refined , N may become very large and the residual type estimator is not used. Instead, we use a reduced Z-Z[12] error estimator.

The Z-Z error estimator[12] is famous one, which was indicated as most robust one by the article [18], in the non-residual type error estimators. The key idea constructing the Z-Z estimator is using information of an element and its neighboring elements to generate the polynomial with higher degree for estimating the discretization error[12]. Below, the reduced Z-Z error estimator based on Z-Z's idea is presented.

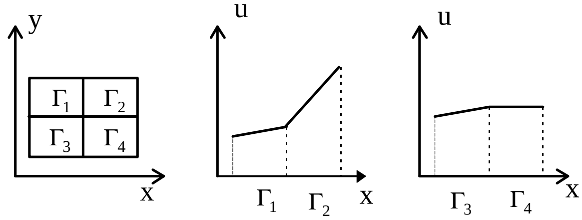


Fig. 4. Variance of *u* on four adjacent elements.

In Fig. 4, the variable *u* on four adjacent boundary elements is analyzed along the x axis. Along the *x* axis, the difference of *u* between elements Γ_1 and Γ_2 is relatively large. This means that only two elements along the x axis are not enough to describe the violent variance of *u* , so Γ_1 and Γ_2 need to be refined. But for elements Γ_3 and Γ_4, there is only little change of *u* along the x axis and it means that Γ_3 and Γ_4 need not to be refined. In the same way, this work is done along the y axis to find which elements among Γ_1、 Γ_2、 Γ_3 and Γ_4 should be refined. Briefly, the refined criterion for boundary element Γ_j can be expressed as:

$$\xi_j = \frac{\int_{\Gamma_j} u \, d\Gamma}{S_{\Gamma_j}} - \frac{\int_{\Gamma'_j} u' \, d\Gamma}{S_{\Gamma'_j}} > \delta \tag{10}$$

where, Γ_j and Γ'_j are the adjacent elements along the x or y axis, S_{Γ_j} and $S_{\Gamma'_j}$ are their corresponding areas, d is a given accuracy requirement. We call the estimator defined in (10) the reduced Z-Z local error estimator. Similarly, the global error estimator of k[th] refinement can be defined as follows:

$$\xi^k = \left(\sum_{j=1}^{N} \xi_j\right) / N \tag{11}$$

It is not difficult to see that computation complexity of the reduced Z-Z estimator is O(N), much faster than residual-type estimator. At the same time, it further reduces computation needed by the original Z-Z estimator[12]. But it should be noted that the reduced Z-Z estimator is not valid in the initial mesh because of too coarse initial mesh to find any adjacent elements. In that case, as we mentioned previously, the residual-type estimator is used.

5 Numerical results

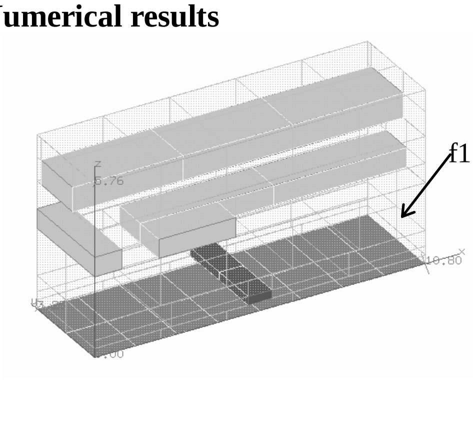
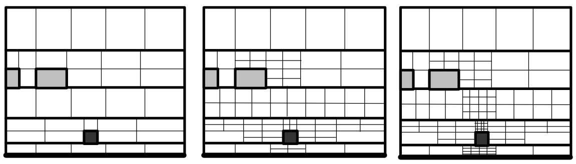


Fig. 5 A parasitic capacitor from practical VLSI layout.

In Fig. 5, the dark conductor is master piece on which the voltage is set 1v and voltages on all the other conductors are set 0v. The grey plane is substrate where its voltage is 0v. The total capacitance to be computed is that between master piece and all other conductors including the substrate. During the adaptive computation, the initial mesh and refined meshes on surface f1 are shown in Fig.6.



(a) Initial (b) First refined (c) Second refined

Fig. 6 Initial mesh and two refined meshes on surface f1.

From Fig.6 , we can see that the error estimator and adaptive tactics based on our algorithm are reasonable. According to the knowledge of electrostatic field, the area between the master piece(voltage=1v) and other conductors(voltage=0v) has great voltage drop. Therefore, the boundary elements near the master should be refined in order to describe the relatively violent variance of electrical potential more precisely. In (b) and (c) of Fig.6, most of the refined elements are just located in neighborhood of the master. The numerical results and electrostatic property match well.

Next, results between the adaptive refinement and uniform refinement are compared for this example. Table 1 shows the results. The capacitance value 674 in Table 1 can be treated as a relatively accurate value by using a very fine mesh.

Table 1 Comparison between h-hierarchical refinement and uniform refinement.

	h-hierarchical		uniform	
	d.o.f.	cap(ff)	d.o.f.	cap(ff)
initial	198	503	198	503
1st ref.	510	623	677	644
2nd ref.	1190	674	2534	670

From above results, we see that in the hierarchical h-adaptive computation using less d.o.f. can reach high precision. But, for uniform refinement, reaching the same precision as the adaptive analysis needs to take much more d.o.f. and additional work, generally.

6 Conclusion

In this paper, the 3-D hierarchical h-adaptive boundary element method is employed to calculate the parasitic capacitance from interconnect in VLSI. The hierarchical computation reduces much work since previous matrix and datum can be reused in the adaptive procedure. The combination of the residual-type estimator and reduced Z-Z error estimator makes error estimation more efficient. Compared with uniform refinement strategy, the adaptive refinement can reach high precision with less degree of freedom.

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