

# Capacitance Extraction from Complex 3D Interconnect Structures

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## Abstract

A new tool has been developed for calculating the capacitance matrix for complex 3D interconnect structures involving multiple layers of irregularly shaped interconnect, imbedded in different dielectric materials. This method utilizes a new 3D adaptive unstructured grid capability, and a linear finite element algorithm. The capacitance is determined from the minimum in the total system energy as the nodes are varied to minimize the error in the electric field in the dielectric(s).

## Summary of Method

The new computational capability allows treatment of multiple dielectric materials, and any shapes for the metal

interconnect and dielectric, and is enabled by a 3D unstructured grid tool recently developed at Los Alamos National laboratory [1]. The key attributes in this new grid tool are:

- unstructured grids to accurately fit any shape;
- accurate treatment of the material interfaces;
- automatic node-redistribution according to a user specified field.

The general characteristics of this capacitance extraction code (Poisson solver) are summarized in Figure 1.

## Solving Poisson's Equation for Complex 3D Structures

### Problem

- Accurate solution of Poisson's equation for complex 3D structures with multiple materials

### Present approach

- 3D adaptive unstructured grids
- Linear finite elements (FE)
- Multiple material properties
- Hybrid and adaptive grids

### Strengths of present approach

- Unstructured grid treats any geometry
- Multiple materials
- Grid adapted (nodes moved) to minimize error in solution gradient
  - eliminates need for higher order FE
- If energy-based formulation, variational minimum can be obtained for fixed number grid points

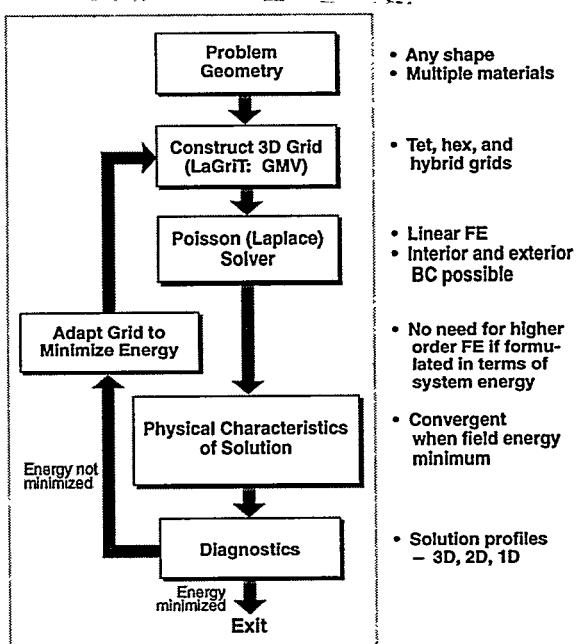


Figure 1

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This new approach gives accurate capacitance results for complex structures with only linear finite elements [as opposed to higher-order finite elements] because the capacitance is extracted from the minimum in the total system energy (Thompson's theorem: Collin [2], Weber [3]) obtained by adapting the grid. That is, the grid node-redistribution process [4] gives a minimum in the total system energy for fixed number of nodes, which then defines an upper limit to the capacitance. As the nodes (fixed number) are re-distributed to minimize the error in the calculated electric field, the system energy reaches a minimum. As more nodes are added, the minimum energy converges to a "best" value, from which the converged capacitance value is obtained.

### Application of the Hybrid Finite Element-Boundary Element Method for Exterior Electromagnetic problems

In capacitance extraction problems the electric conductors are embedded in a possibly inhomogeneous and/or anisotropic dielectric material in a small region of space outside of which one can assume homogeneity, isotropy, and the presence of no changes. The goal is to solve the Poisson equation for the whole space with appropriate boundary conditions in the asymptotic region. For a general geometry of conductors and dielectric material there is no boundary condition available at a surface around the small region of interest. On the other hand to solve the Poisson equation for the whole space is an arduous and undesirable job. Fortunately, due to the homogeneity and isotropy outside of small region, the asymptotic boundary conditions for the potential can be replaced by a constraint on the potential and its derivative on an arbitrary surface. Physically, this means that the actual problem can be replaced by a one where some charges have been introduced on a boundary surface. This modified problem can then be solved via a combination of the finite element method (FEM) inside the surface and the boundary element method (BEM) on the surface. Following McDonald and Wexler [5] the following procedure can be implemented. Inside the bounding surface the Poisson equation for the potential,  $\phi$ , is solved.

$$-\bar{\nabla} \cdot (\epsilon \bar{\nabla} \phi) = \rho \quad (1)$$

via the FEM. On the bounding surface, the potential also satisfies the following identity

$$\phi(\bar{r}) = 2 \int_S \left[ (G(\bar{r}, \bar{r}') \frac{\partial \phi(\bar{r}')}{\partial n'} - \phi(\bar{r}') \frac{\partial G(\bar{r}, \bar{r}')}{\partial n'} \right] \quad (2)$$

where  $S$  is the surface,  $\partial \phi / \partial n'$  is the directional derivative of  $\phi$  along the bounding surface, and  $G(\bar{r}, \bar{r}')$  is the free-space Green's function,

$$G(\bar{r}, \bar{r}') = \frac{1}{\epsilon} \frac{1}{|\bar{r} - \bar{r}'|}. \quad (3)$$

If a system of nodes (inside the surface and on the surface) is introduced, then the FEM can be used inside, and the BEM on the surface. The latter gives a linear relationship between the node-potentials on the boundary to those inside the boundary. This relationship allows one to eliminate the node-potential on the boundary from the problem and reduce it to a problem only for the node-potentials inside the boundary surface [5]. In the numerical implementation of this method, integrals of the type:

$$\int_{S_j} \alpha(\bar{r}') \frac{1}{|\bar{r} - \bar{r}'|} ds', \quad \int_{S_j} \alpha(\bar{r}') \bar{\nabla} \frac{1}{|\bar{r} - \bar{r}'|} ds' \quad (4)$$

are calculated, where  $S_j$  is an element on the surface  $S$  and  $\alpha$  is a node function of a node on the surface. The calculation of the above integrals, if done numerically, leads to singularities which, however, can be avoided if they are calculated analytically following Graglia [6].

### Grid Adaption Using the Minimum Error Gradient Method

The Minimum Error Gradient Adaption (MEGA) is a generalization of the 2D adaptive smoothing scheme of Bank and Smith [7], combined with the *gradient weighting* concept of Carlson and Miller [8]. The idea is to adjust the positions of the vertices so as to minimize the functional.

$$F = \int \|\nabla(u - u_L)\|^2 w dx. \quad (5)$$

That is, the functional is the weighted  $\ell_2$  norm of the gradient of the error between the true solution  $u$  and its piecewise linear approximation  $u_L$  on each tetrahedron. Minimizing the gradient of the error leads to optimal resolution of solution gradients which can be crucial for correct calculation of various physical fields. A secondary benefit of minimizing the error gradient is that it works to prevent "tet collapse" as the mesh moves. This is because solution gradients are poorly represented on wafer-thin tetrahedra and are thus avoided when minimizing this functional. For sufficiently large grids, the gradient weighting factor  $w$  can be omitted and the grids produced become independent of the scale of  $u$ , thus eliminating the necessity of adjusting parameters.

Since the exact solution  $u$  in (5) is generally unknown, the method is to approximate the error by the six quadratic "bump" functions associated with the edges of each tetrahedron. The "bump" functions are the pairwise products of the four linear "hat" functions associated with the four vertices of each tetrahedron.

The LaGriT code also has a novel 3D algorithm for re-establishing Delaunay triangulation after node movement. This algorithm performs internal face swaps and boundary edge swaps in the mesh which typically modify a small proportion of the mesh connectivity during any given time step. As is well known, maintaining a Delaunay grid at all

times is a crucial requirement for many finite volume PDE solvers.

Figure 2 illustrates the adaption of the grid so as to minimize the error in the electric field for the case of a single charged spherical conductor, as described in the next section.

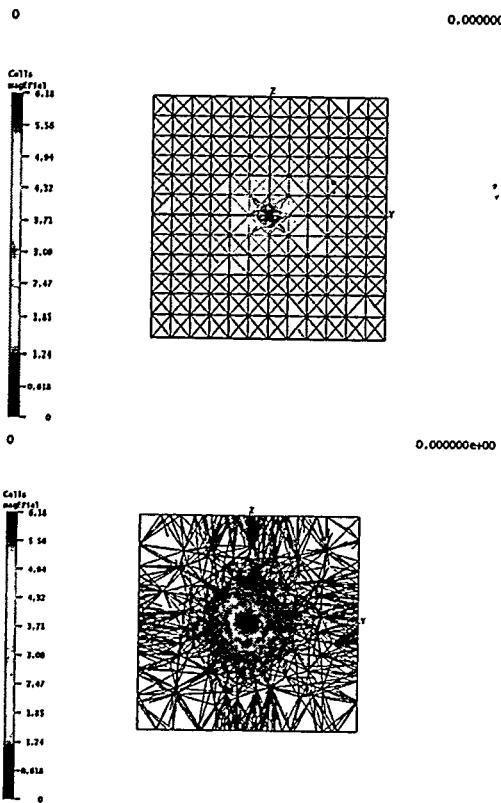


Figure 2. Sequential images of the grid as it is adapted to minimize the error in the electric field. Both images are of a "slice" in the  $yz$ -plane just the thickness of the sphere. Upper figure is the initial grid and the lower figure shows the converged (capacitance minimum) achieved after the fifth grid adaption.

## Results

Figure 3 shows results for the capacitance as a function of the number grid adaptions (left panel), parametric on the number of grid points. The analytical exact result is shown as the horizontal dashed line. These results illustrate how the method converges to a minimum (upper limit) in the system capacitance, for a fixed number of nodes, as the nodes are moved. The right panel illustrates how a simple first-order rational function extrapolation provides the result that would be obtained as the number of nodes goes to infinity. The upper curve in the right panel illustrates the capacitance obtained if no grid adaptation is used (taken from the points for # of adaptions = 0 in left panel.)

CIC-198-1416 (9-98)  
**Test Case - Infinite Spherical Capacitor**  
[ $R = 0.1$  m,  $V = 1.0$  volts] ( $C = \text{exact} = 4\pi\epsilon_0 R$ )

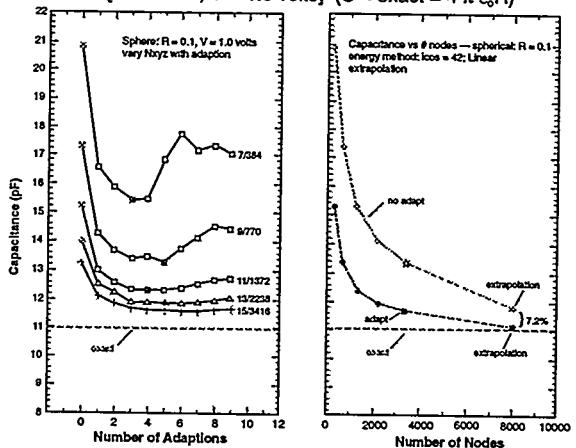


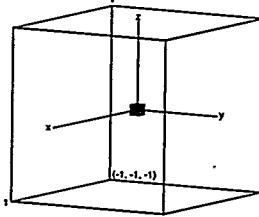
Figure 3

Figure 4 illustrates the results for the test case an infinite cubical capacitor for which there is an "exact" numerical result as shown in this figure. The interpretation of the left and right panels in this figure is the same as in figure 3.

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## Capacitance Extraction

**Test Case - CUBE**  
**Side = 0.1 m**  
 **$V = 1.0$  volts**



Exact (7.283 pF) given by  
D.K. Reitan and T.J. Higgins  
J. Appl. Phys. 22, 223 (1951)

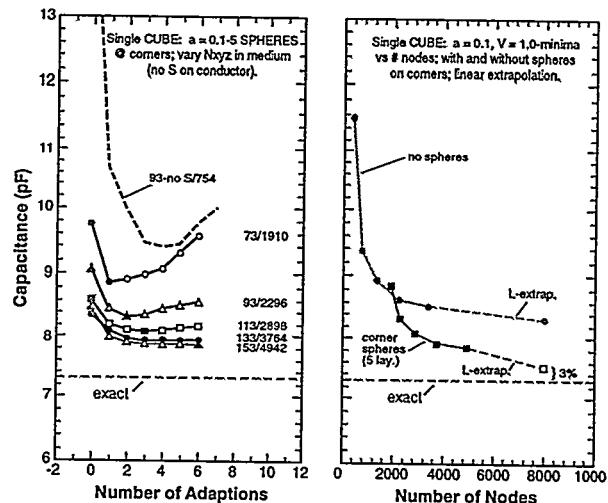


Figure 4. Test case of infinite cubical capacitor. See test for discussion.

Figure 5 shows isocontours of the electric field for the case of 15 grid points in the x, y and z directions (3,416 nodes) and illustrates the concentration of the electric field at the eight corners of the cube addressed in [Figure 4].

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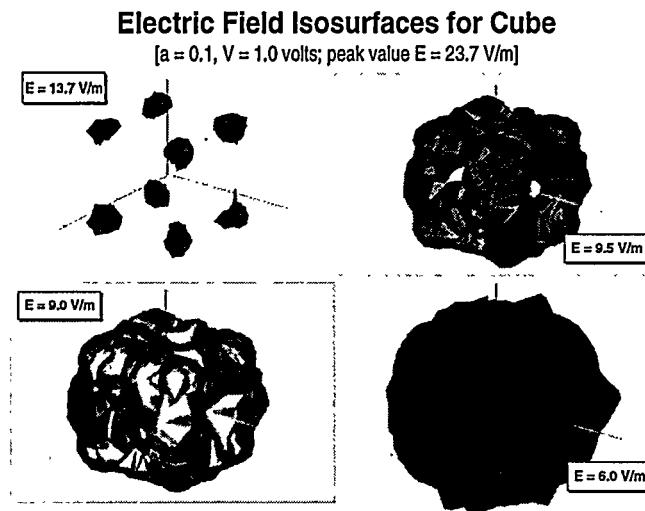


Figure 5. Isocontours of the electric field for a cubically-shaped conductor.

Additional test cases, involving multiple dielectrics will be discussed during the meeting.

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