Simple APDL implementation of a 3D FEM simulator for mutual capacitances of arbitrarily shaped objects like interconnects

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ABSTRACT

This paper describes the implementation of an ANSYS Parametric Design Language (APDL) macro called CAMACO for the computation of capacitance matrixes of arbitrarily shaped 3D objects in arbitrarily distributed dielectrics via the conservation of field energies. APDL as the interface language of the general purpose FEM system ANSYS-Multiphysics™ provides an exceptional high level of abstraction and enables the realization with acceptable effort. The most significant advantage of the described implementation is the utilization of the advanced 3D capabilities of ANSYS™ to generate, edit and visualize realistically shaped ('non-Manhattan') 3D structures either by parametric description and/or graphical interaction (e.g. spaceball; VRLM models etc.) exceeding known solution. These features are especially helpful for initial principal design studies of potential structures.

One typical application of CAMACO is the computation of capacitance matrixes for parasitic elements in DRAM memory cells. A 3D multi-level metal interconnect capacitance analysis of a potential trench capacitor 1GBit DRAM cell in 150nm minimum feature size is discussed.

Keywords: Capacitance simulation, 3D FEM, Interconnect, ANSYS, APDL

INTRODUCTION

The exact computation of parasitic electric capacitances of interconnects within integrated structures especially deep sub-micron ULSI and microsystems has become a crucial part of the design and performance prediction. A variety of numerical methods and algorithms for the computation of electrostatic field problems and the subsequent calculation of capacitances of 2D and 3D geometries have been repeatedly reported in the past. Several programs are known which can compute mutual capacitances. However, most of them provide limited capabilities in terms of fast interactive 3D model generation and visualization. Furthermore the simulation of realistically smooth-shaped objects is rarely possible.

In general, this may be due to the additional effort required to create an advanced 3D interface compared to the effort for the realization of the capacitance computation module it self.

THEORETICAL BACKGROUND

A pure electrostatic system is governed by the Maxwell equation

$$\iiint_v \rho \, dv = \varepsilon_r \varepsilon_0 \oiint \vec{E}(\vec{r}) \, d\vec{A} \qquad (1)$$

(Gauss's law) and the derivable Poisson equation

$$\varepsilon_0 \nabla\left[(\varepsilon_r(\vec{r}) \, \nabla\varphi(\vec{r})\right] = -\rho(\vec{r}) \ . \qquad (2)$$

For the given problem dielectrics may be distributed arbitrarily but no space charge effects apply. In a system of n conductors the charge Q_i on each conductor i for a given set of boundary conditions can be calculated by means of the capacitance matrix

$$Q_i = \sum_{j=1,\ j\neq i}^{n} C_{ij} \, U_{ij} \qquad (3)$$

taking into account the voltage difference U_{ij} between each conductor i and the remaining (n-1) conductors. Due to this definition and the physical nature of the problem the coefficients, C_{ij} , follow three restriction:

The matrix is (I) square, (II) symmetrical and (III) the diagonal elements are equal to the sum over the remaining elements in a line

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

Therefor the number of really unknown values is

$$n_{cap} = \frac{n(n-1)}{2} \ . \qquad (5)$$

These values represent the mutual capacitances while the C_{ii} represent the derivable self capacitance values.

To calculate the charge on a conductor one could use Equation (1) and integrate the electrical field over the closed surface of each conductor

$$Q_i = \varepsilon_r \varepsilon_0 \oiint \vec{E}(\vec{r}) \, d\vec{A}_i \ , \qquad (6)$$

usually referred to as principle of charge conservation. However, for numerical reasons a far more accurate and computationally simpler way is to apply the principle of energy conservation using the electric field energy stored in a given field configuration and determined by the boundary conditions

$$W = \tfrac{1}{2}\,\varepsilon_0 \iiint_V \varepsilon_r(\vec{r})\,[\nabla\varphi(\vec{r})]^2\,dV \qquad (7)$$

which can be simplified by recognizing that

$$W = \tfrac{1}{2}\,\varepsilon_0 \iiint_V \varepsilon_r(\vec{r})\,\left[\vec{E}(\vec{r})\right]^2\,dV \qquad (8)$$

which simplifies to

$$W = \tfrac{1}{2} \iiint_V \vec{E}(\vec{r})\,\vec{D}(\vec{r})\,dV \,. \qquad (9)$$

Eq. (7)-(9) apply in general to arbitrarily distributed dielectrics. Furthermore, the relation

$$W = \tfrac{1}{2}\,C\,U^2 \qquad (10)$$

is used to set up a linear system of equations with n_{cap} unknowns containing the squares of the voltage differences $\tfrac{1}{2}\cdot_k U_{ij}^2$ and the respective field energies, W_k ,

$$\begin{bmatrix} \tfrac{1}{2}_1U_{12}^2 & \tfrac{1}{2}_1U_{13}^2 & \tfrac{1}{2}_1U_{14}^2 & \tfrac{1}{2}_1U_{23}^2 & \tfrac{1}{2}_1U_{24}^2 & \tfrac{1}{2}_1U_{34}^2 \\ \tfrac{1}{2}_2U_{12}^2 & \tfrac{1}{2}_2U_{13}^2 & \tfrac{1}{2}_2U_{14}^2 & \tfrac{1}{2}_2U_{24}^2 & \tfrac{1}{2}_2U_{24}^2 & \tfrac{1}{2}_2U_{34}^2 \\ . & & & & & . \\ . & & & & & . \\ . & & & & & . \\ \tfrac{1}{2}_6U_{12}^2 & . & . & . & . & \tfrac{1}{2}_6U_{34}^2 \end{bmatrix} \cdot \begin{bmatrix} C_{12} \\ C_{13} \\ C_{14} \\ C_{23} \\ C_{24} \\ C_{34} \end{bmatrix} = \begin{bmatrix} W_1 \\ W_2 \\ W_3 \\ W_4 \\ W_5 \\ W_6 \end{bmatrix} \qquad (11)$$

here exemplified for a 4-body system with 6 unknowns. A set of $k=1\ldots n_{cap}$ linear independent vectors containing the squares of the voltage differences $\tfrac{1}{2}\cdot_k U_{ij}^2$ has to be created ensuring that that the determinant of the resulting matrix is non-zero. The n_{cap} energies W_k of the respective field distributions are the quantities to be calculated.

Using the linear nature of the problem, it is only necessary to calculate n direct field solutions obtained from n orthogonal boundary condition vectors and to generate the remaining n_{cap}-n solution by superposition. In general, it would be sufficient to calculate the $\vec{E}(\vec{r})$ and $\vec{D}(\vec{r})$ fields after the superposition from $\varphi(\vec{r})$ and $\varepsilon_r(\vec{r})$. However, this approach, while requiring less memory storage, faces certain practical problems. Therefor the $\vec{E}(\vec{r})$ and $\vec{D}(\vec{r})$ fields from the first n field solutions are stored and not $\varphi(\vec{r})$. The first $k=1\ldots n$ field energy values are obtained by

$$W_k = \frac{1}{2}\sum_{l=1}^{n_{element\_max}} \sqrt{E_{x\,k,l}^{\,2} + E_{y\,k,l}^{\,2} + E_{z\,k,l}^{\,2}} \cdot \sqrt{D_{x\,k,l}^{\,2} + D_{y\,k,l}^{\,2} + D_{z\,k,l}^{\,2}} \cdot v_{elem\ l} \qquad (12)$$

and the remaining n_{cap}-n solutions require superposition

$$W_k = \frac{1}{2}\sum_{l=1}^{n_{element\_max}} \sqrt{\left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} E_{x\,k,l}\right]^2 + \left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} E_{y\,k,l}\right]^2 + \left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} E_{z\,k,l}\right]^2} \cdot \sqrt{\left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} D_{x\,k,l}\right]^2 + \left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} D_{y\,k,l}\right]^2 + \left[\sum_{\substack{l=1 \\ \forall U(l\neq 0)}}^{n} D_{z\,k,l}\right]^2} \cdot v_{elem\ l} \qquad (13)$$

Equation (11), with the actual number of n_{cap}, is solved via a single APDL command and the capacitance matrix C_{ij} is filled by obtaining the C_{ii} via (4) and using the symmetry condition.

PRACTICAL ASPECTS

Two version of CAMACO for 2D and 3D problems exist. User input (from an input script or command line) is a sequence of commands that defines the number of bodies (volumes or areas) and their reference number which will then be considered as the bodies for which the capacitance matrix has to be calculated.

However, a user must be aware of the model generation principles of ANSYS™ since creating and meshing of a model is in general more complicated than in classical capacitance simulation programs like e.g. RAPHAEL™ (TMA/Avant!) or Clever™ (Silvaco) but on the other hand also significantly more flexible and interactive.

The results presented in the next section have been obtained under WindowsNT™ 4.0 on a Dual-PentiumII™ 400MHz machine with 1Gbyte RAM and an Intergraph™ Intense 3D Pro 3410 graphics accelerator. To run jobs with resolutions necessary for realistically shaped 3D objects at least 512Mbyte RAM are advisable.

Among the variety of provided ANSYS™ solvers the Preconditioned Conjugate Gradient solver has been used due to its speed; single electrostatic 3D problems with 10^6 unknowns have been solved in less than 1hour.

COMPUTATIONAL RESULTS

It is generally complicated to determine the precision of results from multi-body capacitance simulations. The systematic evaluation of the numerical behavior remains crucial to establish a trustworthy tool. Only few cases with analytical solution for the capacitance of two conductors are known. More complicated models can only be judged by observing the convergence behavior and correct transfer of physical symmetry of the model to symmetry of the capacitance matrix. For these tests, artificial and highly symmetrical models are preferred since "real" structures contain excessive complexity to determine reasons for usually observed differences in results between different programs operating on the same input model. The functionality of CAMACO has been verified by comparison with results from other programs for a variety of 2D and 3D multi-body cases. For brevity, only two very simple examples can be given thereafter.

One of the few problems with known analytical solution consists of **two infinite long cylinders** with different radii r_1 and r_2 in a distance d within a surrounding dielectric:

$$\frac{C}{l} = \frac{2\pi\varepsilon_0\varepsilon_r}{\cosh^{-1}\left(\dfrac{d^2 + r_1^{\,2} - r_2^{\,2}}{2dr_1}\right) + \cosh^{-1}\left(\dfrac{d^2 - r_1^{\,2} + r_2^{\,2}}{2dr_2}\right)} \qquad (14)$$

As **example 1** the parameters were chosen:
$r_1 = 0.25\mu m$ $r_2 = 0.15\mu m$ $d = 0.660424919\mu m$ $\varepsilon_r = 4.0$ and simulated with CAMACO and RAPHAEL™. The

expected result is $C / l = (1 + 2\cdot10^{-9}) \cdot 10^{-10}$ F/m. As shown in Fig. 1, absolute values of relative errors for results obtained by applying Eq. (12) on the order of $|\Delta C/C| \approx 10^{-3}$ can be achieved. Even with almost the minimal possible number of nodes per conductor in order to represent its shape errors in the order of $|\Delta C/C| \approx 10^{-2}$ are possible. In a special computation mode, using the intrinsic EDENS function not discussed here and applicable only to two-body cases, errors smaller than $|\Delta C/C| < 10^{-4}$ can be reached.

The **second** simple **example** assembles **three cubes** $m_1 \ldots m_3$ each with $V=1\mu m^3$ in a distance $d=2\mu m$ of their centers in a large fourth cube m_4 with $V=40\mu m^3$, $\varepsilon_r=1$ and Neumann boundaries as shown in Fig. 2. Results were again calculated with CAMACO and RAPHAEL™ for different discretizations and are show in Fig. 3. Remarkably and very useful for practical applications, CAMACO again achieves more rapid convergence to solutions for DOF$\rightarrow\infty$.

Finally, Fig.4 illustrates the application of CAMACO in a 3D multi-level metal interconnect capacitance analysis of a potential trench capacitor 1Gbit DRAM cell with 150nm minimal feature size. Crucial in DRAM cells is the bitline capacitance determining the transfer ratio and therewith limiting the maximal possible number of cells per bitline. Typical models consist of $5\cdot10^4$ to $2\cdot10^5$ nodes and 8 to 12 interconnects are considered as bodies for the capacitance matrix. Note the realistic shape of the bitline studs in Fig.4.

SUMMERY

An APDL macro has been described for the computation of mutual capacitances of arbitrarily shaped 3D objects which can be used for ULSI, microsystems, packaging, MCMs, printed boards and transmission lines. Extended investigations revealed, that it is possible achieve precision on the order of $|\Delta C/C| \approx 1\cdot10^{-2}$ for practical problems. CAMACO can be used on any platform running ANSYS™: AIX™, Digital Unix™, HP-UX™, IRIX™, Solaris™, UNICOS™ and WindowsNT™.

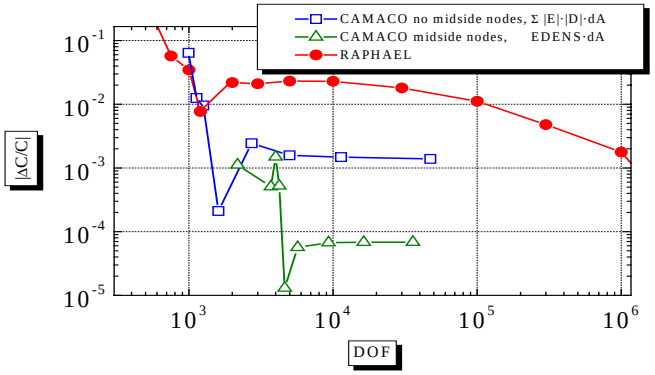

Fig. 1 CAMACO and RAPHAEL™ results for example 1: absolute value of relative error of *C/l* as function of DOF (number of grid-points respectively for RAPHAEL™ results); Curve 1: standard use of ANSYS Element Plane121 without midside nodes and applying Eq.(12); Curve 2: maximal precision with Element Plane121 with midside nodes and use of intrinsic EDENS function (only applicable to two-body problems)

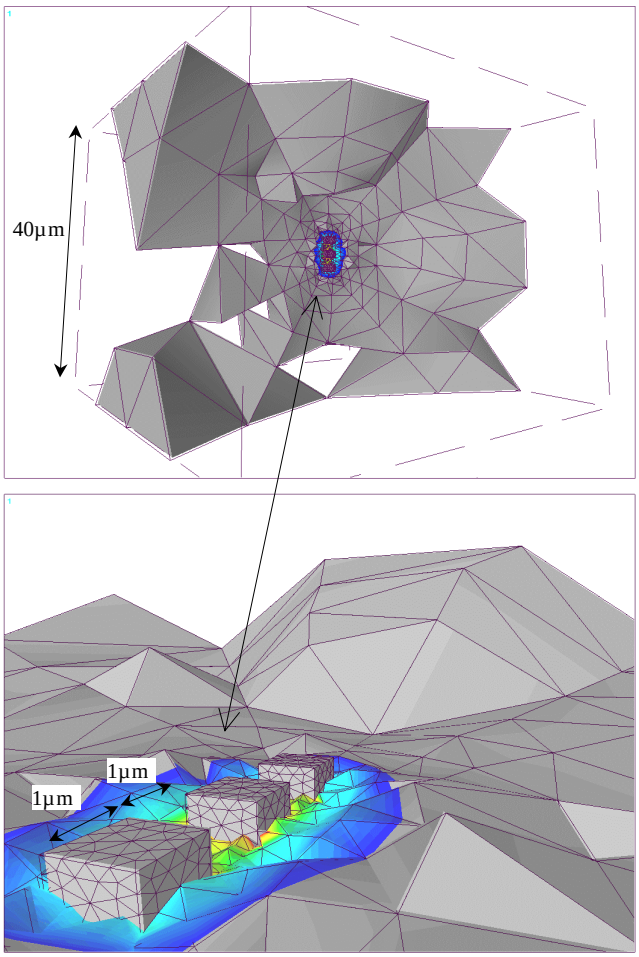

Fig. 2 Example 2: Capacitances of the three cubes $V=1\mu m^3$ in $d=2\mu m$ distance to each other inside a large fourth cube $V=40\mu m^3$ representing the surrounding free space with Neumann boundaries on the outer areas; most elements have been removed to enable visibility; bottom: contour plot of absolute electric field strength in vicinity of cubes

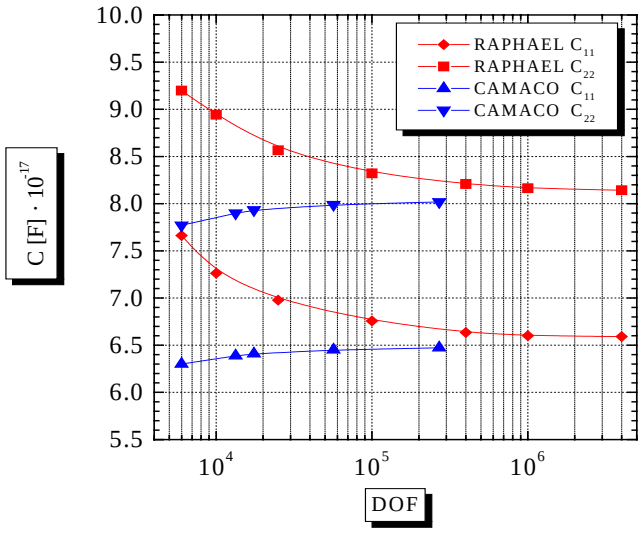

Fig. 3 Absolute values of C_{11} and C_{22} for reference example 2 in Fig. 2 as a function of number of DOF (number of grid-points respectively) obtained from CAMACO and RAPHAEL™

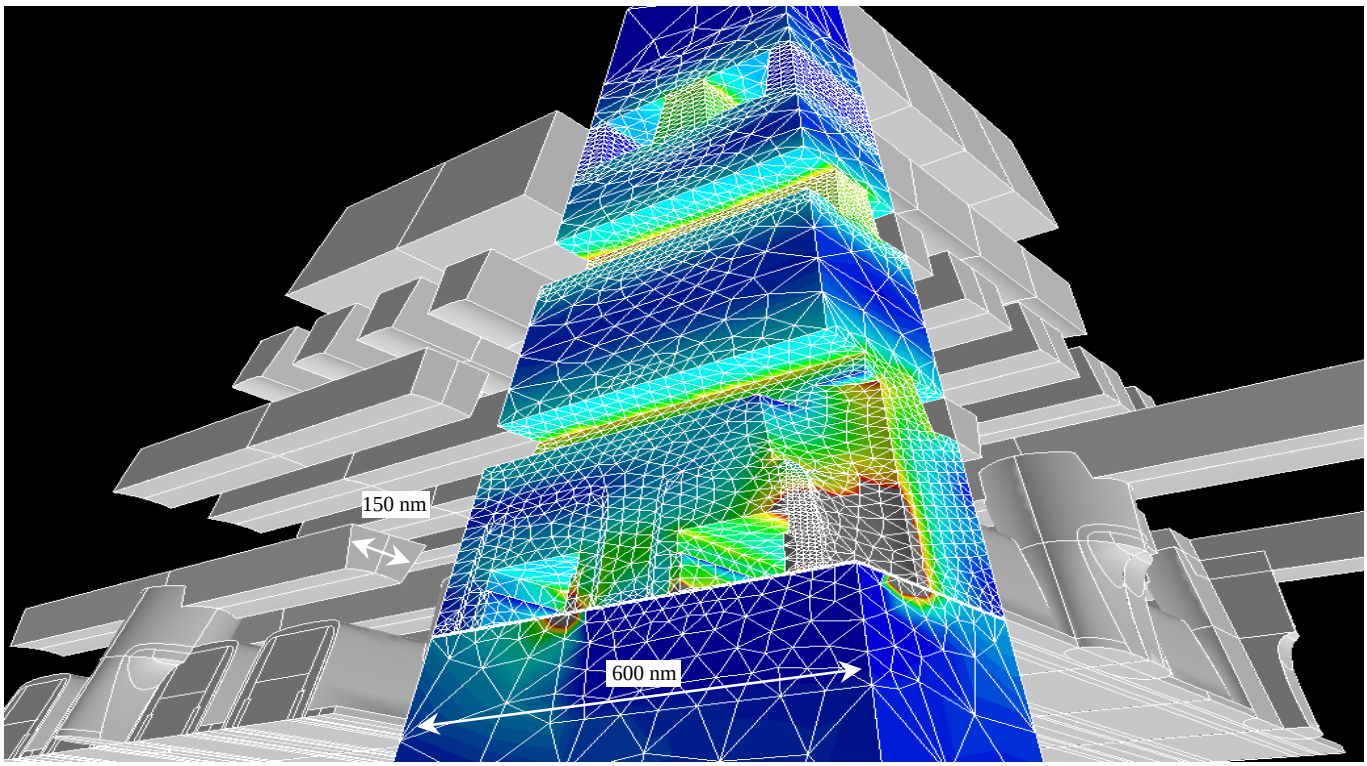

Fig. 4 Application of CAMACO/ANSYS™ in a 3D multi level metal interconnect capacitance analysis of a potential trench capacitor 1GBit DRAM cell with 150nm minimum feature size; elements and contour plot of absolute electric field strength in dielectrics of unit cell, metals and some liner volumes; model consists of approximately 120,000 nodes; [9×9] capacitance matrix

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