Computation of Second Order Capacitance Sensitivities Using Adjoint Method in Finite Element Modeling

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Abstract — The sensitivities of capacitance to the design parameters can be computed by either the derivative of potentials or the adjoint variables. By using the variational method for the electric flux computation, it can be shown that the right hand side of the adjoint system is identical to the right hand side of the original system. In combining the two methods, the second order sensitivities can be computed with reduced cost. First and second order derivatives of material matrix are accomplished with the help of the first and second order local jacobian derivatives.

I. INTRODUCTION

The sensitivity of the circuit elements to the design or process parameters has a great importance in the design, optimization and manufacturing of electrical and electronic devices. For example, in nano-scale IC systems, the sensitivity analysis helps the prediction and diagnosis of the system failure resulting from the variation, perturbation and uncertainty of the fabrication process and guides the robust design optimization to ensure the reliability and to increase the yield.

In the extraction and characterization of the circuit parameters using the numerical technique such as the finite element method, it is well known that the computation of sensitivities via explicit derivative such as the differential method is expensive and inaccurate. Two methods can be applied to avoid the direct derivative using the differential method. One is to compute the sensitivity (derivatives) of the working variables. The other is to use the adjoint technique.

The adjoint circuit method has been used to analyze the circuit sensitivities since about four decades [1][2]. It has also been applied in high frequency electromagnetic field analysis for the sensitivities of the circuit parameters [3][4][5]. In the case of scattering matrix of a multiport microwave device using edge element, it has been shown that the adjoint solution can be obtained from the field solution [3], which reduces the computation cost. Computation of sensitivities of working variables consists of solving the system equation with the right hand side the product of the derivative of the system matrix and the existing solution. This procedure can be easily accomplished with the help of the local jacobian derivative [6].

The majority of previous work focuses on the first order sensitivities. However, in the systems which involve large variations, the first order sensitivity appears insufficient. The second order sensitivity becomes necessary. In this paper, we combine the two techniques to compute the second order capacitance sensitivities to the design or process parameters.

II. ELECTROSTATIC FIELD AND CAPACITANCES

To compute the capacitances of a multi-conductor system, we solve first the electrostatic field problem. The finite element discretization leads to the following matrix equation in terms of electric potential v:

$$\mathbf{M}(\mathbf{p})\mathbf{v} = \mathbf{S},\tag{1}$$

where the material matrix M is a function of the design (geometry or material) parameters, noted by p, and S the right hand side resulting from enforced Dirichlet condition.

To compute the capacitance matrix of an n-conductor system, the system equation (1) is solved n-1 times, by applying respectively, one volt voltage excitation on one conductor and zero volt voltage on others.

The capacitance between the conductor i and j (C_{ij}) is computed by integrating the electric flux on a surface surrounding the conductor j (which equals the electric charges containing in the conductor). Since the continuity of electric flux is weak in the formulation (1), it appears more convenient and accurate to compute the electric flux via the variational way [7]. Let's denote by F_{ij} the electric flux around the conductor j with the excitation on the conductor i, we have

$$F_{ij} = \sum \left((Mv)_n : n \in \Gamma_{ej} \right), \tag{2}$$

where n is the node number. $(Mv)_n = 0$ except for the set of nodes belonging to Γ_{ej} , the boundary of conductor j. For a unit excitation on the conductor i, F_{ij} is in fact the capacitance C_{ij} we look to compute. The expression (2) can be written in the matrix form:

$$\mathbf{C}_{ij} = \mathbf{k}_{j}^{\mathrm{T}} \mathbf{M} \mathbf{v} \,, \tag{3}$$

where k_j is a vector with unit entries for $n \in \Gamma_{ej}$ and zero elsewhere, and v is the potential solution with unit excitation on the conductor i.

III. COMPUTATION OF FIRST ORDER SENSITIVITY

There are two ways to compute the capacitance sensitivity. One is to compute the derivative of potential v, the other is solving adjoint equation.

Taking the derivative on both sides of equation (1) with respect to a design (geometry) parameter p_l , we have

$$M\frac{\partial v}{\partial p_1} = -\frac{\partial M}{\partial p_1}v.$$
(4)

If we know how to compute $\partial M/\partial p_1$, once we get the solution v from (1), we can compute the right hand side of (4) and solve the linear matrix system equation (4) to get $\partial v/\partial p_1$. The capacitance sensitivity can be then obtained by

taking the derivative of eq. (3):

$$\frac{\partial \mathbf{C}_{ij}}{\partial \mathbf{p}_{1}} = \mathbf{k}_{j}^{\mathrm{T}} \left(\frac{\partial \mathbf{M}}{\partial \mathbf{p}_{1}} \mathbf{v} + \mathbf{M} \frac{\partial \mathbf{v}}{\partial \mathbf{p}_{1}} \right).$$
(5)

For a system with m design parameters, equation (4) needs to be solved m times. It can be noted that matrix in (4) is exactly the same as in (1). In the case of solving (1) with the direct method, the solution of (4) can be simply obtained by the matrix-vector product. However, when solving the system equation using the iterative method, solving (4) multiple times may become expensive.

An alternative way to compute the sensitivity is to use the adjoint method. Taking the derivative of C_{ij} with respect to the potential v as the right hand side, we get the following adjoint system:

$$M u = \frac{dC_{ij}}{dv}, \qquad (6)$$

where u is the adjoint variable, and the right hand side, according to (3), is given by

$$\frac{dC_{ij}}{dv} = k_j M .$$
(7)

After solving (6) and considering the relationship

$$\frac{\partial C_{ij}}{\partial p_1} = \left(\frac{dC_{ij}}{dv}\right)^1 \frac{\partial v}{\partial p_1}, \qquad (8)$$

the capacitance sensitivity is obtained by

$$\frac{\partial C_{ij}}{\partial p_1} = \mathbf{u}^{\mathrm{T}} \mathbf{M} \frac{\partial \mathbf{v}}{\partial p_1} = -\mathbf{u}^{\mathrm{T}} \frac{\partial \mathbf{M}}{\partial p_1} \mathbf{v}, \qquad (9)$$

providing $\partial M / \partial p_l$ is pre-computed.

It can be noted that the right hand side of the adjoint equation (6), or eq. (7) per say, is nothing else but the right hand side of the original equation (1) with the unit voltage excitation on the conductor j. The solution of the adjoint variable u in (6) is hence the solution of the original equation which exists already when compute the full capacitance matrix of the multi-conductor system. The sensitivities of capacitance can be in that case computed for free. Here we reach the similar observation as in [3].

IV. SECOND ORDER SENSITIVITY

Taking derivative of equation (4) with respect to a design parameter p_m , we get

$$\mathbf{M}\frac{\partial^2 \mathbf{v}}{\partial \mathbf{p}_1 \partial \mathbf{p}_m} = -\frac{\partial \mathbf{M}}{\partial \mathbf{p}_m}\frac{\partial \mathbf{v}}{\partial \mathbf{p}_1} - \frac{\partial^2 \mathbf{M}}{\partial \mathbf{p}_m \partial \mathbf{p}_1}\mathbf{v} - \frac{\partial \mathbf{M}}{\partial \mathbf{p}_1}\frac{\partial \mathbf{v}}{\partial \mathbf{p}_m} \,. \tag{10}$$

Knowing the potential v and the derivatives of potential to different geometry parameters, we can solve (10) to get the second order derivatives $\partial^2 v / \partial p_l \partial p_m$. This might be however an expense procedure if the number of geometry parameters is important.

To reduce the computation cost, we can use again the adjoint method. Taking the derivative of (9) with respect to p_m , we have

$$\frac{\partial^{2} C_{ij}}{\partial p_{1} \partial p_{m}} = -\left(\frac{\partial u^{T}}{\partial p_{m}} \frac{\partial M}{\partial p_{1}} v + u^{T} \frac{\partial^{2} M}{\partial p_{m} \partial p_{1}} v + u^{T} \frac{\partial M}{\partial p_{1}} \frac{\partial v}{\partial p_{m}}\right).$$
(11)

In (11), the potential v is obtained by solving eq.(1), the derivatives of the potential are obtained by solving (4) and the adjoint variable u is given by (6), which is the existing solution of (1) for full capacitance matrix solution of the multi-conductor system.

The first and second order derivatives of material matrix M with respect to the design parameters p in (4), (9) and (11) are accomplished with the help of the first and second order local jacobian derivatives.

V. EXAMPLE OF COMPUTATION

The present method is validated by computing the capacitances of a three-conductor system. Fig. 1 compares the capacitances obtained by the finite element method and by the first and second order sensitivities, when the width of a conductor varies from 0.2um to 0.4um. It can be seen that results with the second order sensitivity approximation matches well the FEM results even for large variation.

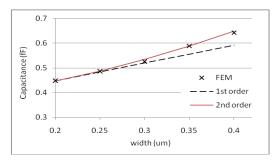


Fig. 1. Capacitance variation in function of width

VI. REFERENCES

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