Submitted to The 17th Annual Review of Progress in Applied Computational Electromagnetics
Session: "Wavelets in Electromagnetics" - Student Paper Competition

Adaptive Numerical Modeling of RF Structures Requiring the Coupling of Maxwell's, Mechanical and Solid-State Equations

N.Bushyager, B.McGarvey and M.M.Tentzeris

(nbushyager@ece.gatech.edu)

School of ECE

Georgia Institute of Technology

Atlanta, GA 30332-250, U.S.A.

Abstract

The FDTD and the Haar-based MRTD algorithms are applied to the full-wave modeling of high-frequency structures that require the combination of differential equations with time-constants of different orders. The numerical coupling of Maxwell's and mechanical equations for the simulation of a MEMS capacitor and of Maxwell's and solid-state equations for a pn diode is discussed in detail.

I. Introduction

State-of-the-art wireless and high-speed computing applications require the effective modeling of complex structures that involve mechanical motion, wave propagation and solid-state effects. Due to computational constraints, most commercial simulators utilize various approximations in order to provide fast and relatively accurate results. The drawback of these approaches is that transient phenomena and nonlinearities are not modeled effectively, leading to the degradation of system-level performance. Alternatively, full-wave techniques provide higher accuracy but suffer from excessive execution time requirements, thus making their efficient numerical implementation very critical. The Finite-Difference Time-Domain technique (FDTD) [1] is one of the most popular and versatile time-domain tools and has been applied to the discretization of Maxwell's equations and of solid-state equations. Lately the MultiResolution Time-Domain technique [2] has provided a mathematically correct way to implement time and space-adaptive gridding, as well as to significantly decrease execution-time and memory requirements. For these reasons, FDTD and MRTD are presented in this paper for the simultaneous modeling of Maxwell's, mechanical and solid-state equations in high-frequency structures.

II. MEMS Structures - Coupling of Maxwell's and Mechanical Equations

II.1 Requirements for MEMS Numerical Modeling

Interest in MEMS technology is growing in the RF field because of the lower loss characteristics of MEMS devices. These loss characteristics translate into higher Q of passive devices, a critical improvement because the Q of embedded passives is a constraining factor for their implementation in many RF technologies. Great strides are being made in the fabrication of MEMS devices, and accurate models of these devices are needed. The numerical simulation of these devices is a difficult proposition for a number of reasons. The first is the need to integrate both mechanical and electromagnetic equations. Most EM simulators are unable to compensate for the changing boundary conditions introduced by the motion of the simulated structure. A second difficulty is the

complexity of modeling their intricate structure. The smallest features of the devices can be several orders of magnitude smaller than the bulk feature size, leading to numerical inaccuracies or very large computational grids. Thus, a simulator for modeling MEMS devices needs to be able to handle moving boundary conditions, the interaction between electrostatic forces and mechanical motion, and difficult to model complex geometries. In the following, a simulator for modeling MEMS parallel plate variable capacitors is discussed.

II.2 MEMS Capacitor

II.2.1. Modeling of Motion

On-chip capacitors are valuable matching and tuning components in most RF circuits. MEMS capacitors have demonstrated very low loss and significantly higher Q in comparison to conventional ones, without increasing space requirements. Modeling of this type of structure is challenging since it has to incorporate the motion of plates under the combined effect of a DC bias and an RF excitation. The model of the capacitor is simplified in order to create a model that will handle many of the features of the MEMS capacitor, while not being overly complex. MEMS capacitors can be fabricated using several different methods, all of which will be constrained and excited in different ways. The capacitor presented herein is a parallel plate capacitor that exhibits one-dimensional motion [3].

The capacitor to be modeled can be seen in Figure 1. It is comprised of two plates, the bottom fixed, the top restrained by a spring and damper. The spring represents the force from the support of the top plate, while the damper represents the resistance of the air. With no applied bias the weight and spring force on the top plate reach equilibrium (the damper only has an effect when the plate is in motion). When a bias is applied, the electrostatic force on the top plate is represented by

$$f = \frac{\varepsilon_\circ A V^2}{(x-h)^2} \tag{1}$$

In this equation, A is the area of the plate, V is the voltage between the plates, h is the initial separation of the plates, and x is the displacement of the top plate from its initial position. This equation neglects fringing fields around the capacitor, and is accurate when the plate size is large compared to the separation. In addition, it is noted that while the voltage is constant, the force changes based on the position of the top plate. In an RF circuit, V varies due to the propagating RF field. When coupled with an electromagnetic simulator, V will vary with time.

The equation of motion of the top plate is the standard 2nd order ordinary differential equation for spring mass systems with (1) as a forcing function. The equation [4] is

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = \frac{\varepsilon_\circ A V^2}{(x-h)^2} \tag{2}$$

The coefficient b is the damping coefficient, k is the spring coefficient, and m is the mass of the plate. In order for the capacitor to operate as desired it must have damped oscillatory motion.

The purpose of this investigation is to combine the mechanical motion of the parallel plate capacitor with a time domain electromagnetic simulator. As such, it would be useful to have a time domain simulation of the capacitor's motion. A finite difference discretization of the above model is now presented. In order to create a model with second order accuracy, central differences are employed.

Using the standard notation

$$u(n\Delta t) = u^n \tag{3}$$

(2) can be written as:

$$m\frac{x^{n+1} - 2x^n + x^{n-1}}{\Delta t^2} = -b\frac{x^{n+1} - x^{n-1}}{2\Delta t} - kx^i + \frac{\varepsilon_\circ A V^2}{(x^n - h)^2} \tag{4}$$

Solving (4) for x^{n+1} gives

$$x^{n+1} = 2x^n\left(\frac{2m - k\Delta t^2}{2m + b\Delta t}\right) + x^{n-1}\left(\frac{b\Delta t - 2m}{b\Delta t + 2m}\right) + \frac{2\Delta t^2 \varepsilon_\circ A V^2}{(2m + b\Delta t)(x^n - h)^2} \tag{5}$$

When implemented, it is assumed that x is equal to zero for all time prior to t=0. This equation could be used by itself to determine the motion of the parallel plate under a fixed bias voltage V. However, it should be noted that V could be varied at any time, and the equation would be able to react to the change. This is very important when combining the equation with an electromagnetic simulator.

II.2.2. Combination with a Time-Domain Electromagnetic Simulator (FDTD, MRTD)

In order to efficiently simulate the motion of the MEMS capacitor under an RF excitation, the above model has to be integrated into an electromagnetic simulator. Two types of full wave time-domain simulators will be discussed, the Finite Difference Time Domain (FDTD) and MultiResolution Time Domain (MRTD) techniques. There are several similarities between these two modeling methods, and some important differences that affect the implementation.

In either type of simulator the plates are represented as metals, the bottom one fixed. The position of the top plate, however, changes with time. Because both simulators are time domain, a change in the boundary conditions, such as would be caused by a moving metal, is not necessarily a problem. Indeed, because the boundary conditions are enforced explicitly at every time step, a moving plate simply causes the boundary conditions to be enforced at different space points for each time step. In this manner, a time varying metal plate is easy to incorporate into an FDTD or MRTD model. In addition, the voltage between the plates caused by the interaction of the capacitor with an applied RF field can readily be calculated from the EM simulator. Thus the bias voltage and voltage due to the applied field can be combined to correctly calculate the forcing function. There are, however, several characteristics of the capacitor geometry that make FDTD modeling difficult.

As stated previously, the separation between the plates is very small compared to their width. In order to accurately simulate the capacitor it is important to have several cells between the plates. This creates a very small cell side length compared to the plate width and the dimensions of any feeding structure. While all three sides of the cell are not required to be the same length, a large aspect ratio between cell side lengths causes numerical inaccuracies. In order to maintain a reasonable ratio between the cell side lengths, the cells used in the simulation must be made very small compared to the computational space. However, the large number of grid points this causes in the simulation are computationally prohibitive. This discretization problem is linked to the dominant difficulty of MEMS modeling, coupling the position results provided by a mechanical simulation to a space-dependent electromagnetic simulation.

The equation of motion (5) is an ordinary differential equation. As such, it is discretized only in time, not space and time. The spatial variable can take on any value. This creates a problem in its integration into the electromagnetic equations, which are discretized in both space and time (as in FDTD and MRTD). In order to simulate the moving metal plate in a fixed spatial grid, the plate must take on one of a discrete number of spatial points. There are at least two ways to handle this difficulty in FDTD. The first method is to find the spatial position of the plate from the motion equation, and apply the plate boundary conditions at the closest grid points. When the motion equation is next updated, the exact computed spatial value would be used for the update. Thus, the electromagnetic simulator would use the averaged values while the motion simulator would not. This would introduce error in several ways.

The first error caused by this method is that the spatial position of the capacitor plate is not exact. The equation for the capacitance of a parallel plate capacitor is

$$C = \frac{\varepsilon_{\circ} A}{d} \tag{6}$$

If d is not represented by a large number of cell widths, the capacitance using the discretized grid points may be unacceptably different from the exact capacitance. These errors would compound during the execution of the problem.

Another option for simulating the capacitor would be to modify the FDTD grid at each time step. The new grid would have a grid level at the exact height of the top plate. The inherent problem with this method is how to determine the field values at the new grid points. Obviously, some type of interpolation would have to be used. The error introduced by this changing grid would be difficult to determine. However, these problems can be alleviated using the adaptive grid provided by MRTD.

MRTD uses a wavelet field discretization. This allows cells to be significantly larger than in FDTD. The resolution of cells that contain fine geometry or high field variation can be increased by locally adding wavelets. These wavelets, which can be both time and space localized, are equivalent to an adaptive grid, which leads to

reduced execution times (areas of small field variation are represented by large cell sizes) and improved memory efficiency. Thus, the MRTD technique can be used with the MEMS motion simulator to resolve the position of the top capacitor plate to any desired level of accuracy. As a rule of thumb, the position of the PEC is updated every 100-500 MRTD/FDTD time-steps and is modeled by zeroing out the appropriate scaling and wavelet coefficients. The maximum wavelet resolution can be determined by the local positioning error of the PEC on the MRTD cell.

II.2.3. Test Capacitor Simulation

In order to test the ability of an FDTD simulator to adequately determine the capacitance of MEMS capacitor, a static MEMS capacitor was modeled. The capacitor used had an area of 450 μm^2, a plate separation of 1 μm, and was fed with a coplanar waveguide over a ground plane. The capacitor was treated as a one port structure, and Γ of the structure was determined. From Γ, the impedance and ultimately the capacitance were determined. The predicted capacitance, using (6), is 1.8 pF. Figure 2 shows a plot of capacitance vs. frequency. As can be seen, the capacitance rises slightly with frequency, and is lower than the predicted value. The change in capacitance with frequency, as well as the lower overall value, is due to parasitics from the feeding structure and the radiation from the capacitor due to fringing fields at the edges. The increasing trend agrees with previously published results [3].

III. Solid-state Structures – Coupling of Maxwell's and Transport Equations

III.1 Transport Equations – Time-step Disparity

The accurate prediction of the performance of high frequency circuits requires the development of a global simulator of Maxwell's and Solid-state equations [5-8]. Most of these approaches involve the simultaneous solution of the Maxwell's equations and of the classic Boltzmann transport equation model that can be written as follows in terms of the majority carrier density n (7), velocity v_d (8), energy w (9), and electric potential φ (10):

$$\frac{\partial n}{\partial t} = \nabla \cdot \left(n \vec{v}_d \right) \tag{7}$$

$$\frac{\partial \left(\vec{v}_d \right)}{\partial t} = -\frac{\vec{v}_d}{m^*} \nabla \cdot \left(m^* \vec{v}_d \right) + \frac{q\vec{E}}{m^*} - \frac{2}{3nm^*} \nabla \left(nw - \frac{1}{2} m^* n \vec{v}_d^{\,2} \right) \tag{8}$$

$$\frac{\partial w}{\partial t} = -\vec{v}_d \nabla \cdot w - \frac{2}{3n} \nabla \cdot \left[\left(n\vec{v}_d - \frac{\kappa}{k_B} \nabla \right) \left(w - \frac{m^* \vec{v}_d^{\,2}}{2} \right) \right] + q\vec{E} \cdot \vec{v}_d \tag{9}$$

$$\nabla^2 \varphi = -\frac{q}{\varepsilon} \left(N_D - n_i \right) \tag{10}$$

n : Carrier Concentration
$\vec{v}_d$: Carrier Velocity
m^* : Carrier Effective Mass
q : Electronic Charge
w : Carrier Energy
φ : Electric Potential
$\vec{E}$: Electric Field
k : Thermal Conductivity
N_D : Majority Carrier Density
n_i : Carrier Concentation
φ : Electric Potential
k_B : Boltzmann's Constant

Initial conditions for the solid-state simulation are provided by the solution of the Poisson equation. Coupling the Maxwell's Equations system to the Solid-state system is accomplished by calculating the voltage applied to the semiconductor and the current injected into the model. The disparity between the time steps required for stable solutions to each independent problem gives numerical difficulties at the interfaces since the time step of the

electromagnetic model is significantly larger than that of the semiconductor model. Simulations performed with a global time step set equal to the smallest of the two values would require unreasonable execution times. However, choosing independent time steps for each set of equations and updating the explicit form of the semiconductor model every FDTD or MRTD time step produces non-physical results, due to the fact that it does not accurately describe the much faster solid-state device response. Dividing the large electromagnetic time step into many smaller time steps appropriate for the semiconductor model and interpolating could accomplish a numerically correct excitation (Figure 3).

III.2 Discretization Issues

Selecting the discretization method for the semiconductor model is challenging. Various approaches of gradually increasing complexity are implemented until stability is satisfactory. Standard notation is presented in (11).

$$\frac{\partial f}{\partial u} = L_u[f], \quad f_i^k = f(x = i\Delta t,\, t = k\Delta t) \tag{11}$$

The first approach used for discretizing all the equations is a central difference in space and a forward Euler difference in time (12). This scheme is simple to implement, but suffers from instability.

$$L_t[f_i] = \frac{f_i^{k+1} - f_i^k}{\Delta t}, \quad L_x[f_i] = \frac{f_{i+1}^k - f_{i-1}^k}{2\Delta x}, \quad L_{xx}[f_i] = \frac{f_{i+1}^k - 2f_i^k + f_{i-1}^k}{(\Delta x)^2} \tag{12}$$

Improving the stability required determining which of the three basic balance equations contributes more significantly to the numerical error leads to approaches that improve the stability. It can be observed that the carrier concentration equation only has convection terms that significantly contribute to the error. The carrier concentration equation has only convection terms, which significantly contributes to the instability. While the forward time and central space scheme is satisfactory for the momentum and energy equations a new discretization method must be found for the carrier equation that will satisfactorily handle the convection nature of the carrier equation. The upwind scheme is commonly used to handle equations with large discontinuities. For this case the

$$\vec{v}_i^k L_x^{up}[f_i] = \begin{cases} \vec{v}_i^k \dfrac{f_i^k - f_{i-1}^k}{\Delta x} & \text{if } v_i \geq 0 \\ \vec{v}_i^k \dfrac{f_{i+1}^k - f_i^k}{\Delta x} & \text{if } v_i < 0 \end{cases} \tag{13}$$

asymmetric nature of the upwind scheme (13) causes unacceptable dispersion in the solution.

The above simple methods have been explored and rejected for the carrier balance equation. A complex method that is commonly used for convection equations is the Lax-Wendroff scheme (14).

$$\vec{v}_i^k L_x^{LW}[f_i] = \vec{v}_i^k \frac{f_{i+1}^k - f_{i-1}^k}{\Delta x} - \frac{(\vec{v}_i^k)^2 \Delta t}{2} \frac{f_{i+1}^k - 2f_i^k + f_{i-1}^k}{\Delta x^2} \tag{14}$$

The Lax-Wendroff scheme provides $O((\Delta t)^2)$ and $O((\Delta x)^2)$ error in time and space. It makes use of a weighted second derivative that introduces diffusion effects into the solution providing additional stability. The complexity of the method increases the computational requirements to find a solution to the balanced equation model (7)-(10).

This model can benefit from MRTD by including wavelets (Figure 4) to the equations that feature fast field/carrier variations or abrupt discontinuities. The carrier balance equation is the natural choice for the addition of wavelets. The Lax-Wendroff scheme had to be used for smoothing the discontinuities in order to achieve stable simulation. Multiresolution techniques can improve the local numerical accuracy by using adaptively more wavelet resolutions where required. Because of this fact, it may be possible to use the simple method of central differences

in space and forward differences in time to accurate model the convection-dominated carrier balance equation without having to use a computationally intensive differencing scheme.

IV. Conclusion

It has been demonstrated that a method for modeling MEMS using existing FDTD techniques, as well as the newer MRTD technique is feasible. The demonstrated technique combines an ODE that describes the motion of the device, as well as time domain simulation of electromagnetic fields. The time domain motion simulation combines well with the time domain electromagnetic simulators. The differences between the simulators are the time steps and discretization. It has been shown that the MRTD technique can be used to compensate for the lack of a discrete space grid in the motion simulation.

Coupling the Solid-state and Maxwell 's equations globally in a single simulator is essential for simulating and designing high-frequency microstructures that include devices such as mixers, LNA's, PA's or other active devices. Simulating semiconductors based on the physical construction of the device can provide insight and optimizations for the design of microstructures prior to fabrication.

References

[1] A. Taflove and S. Hagness, *Computational Electrodynamics, the finite difference time domain approach*, 2nd ed., Boston, Artech House, 2000.

[2] E.Tentzeris, R.Robertson, A.Cangellaris and L.P.B.Katehi, "Space and time adaptive gridding using MRTD", *Proc. of the 1997 IEEE Symposium on Microwave Theory and Techniques*, pp.337-340, Denver, CO.

[3] A. Dec and K. Suyama, "Micromachined electro-mechanically tunable capacitors and their Applications to RF IC's," *IEEE Trans. Microwave Theory Tech.*, vol. 46, no. 12, pp.2587-2596, Dec 1998.

[4] W. Boyce and R. DiPrima, *Elementary Differential Equations and Boundary Value Problems*, 6th ed., New York, J. Wiley and Sons, 1997.

[5] H.-P.Tsai,R.Coccioli and T.Itoh, "Time Domain Global Modeling of EM Propagation in Semiconductor Using Irregular Grids", Proc. IMS2000, pp.367-370, June11-16, Boston

[6] S.M.S. Imtiaz and S.M.El-Ghazaly, "Global Modeling of mm-wave circuits: EM simulation of amplifiers", IEEE-MTTT, vol.45, pp.2208-2216, Dec.1997

[7] S.Goasguen and S.M.El-Ghazaly, "Interpolating Wavelet Scheme Toward Global Modeling of microwave Circuits", Proc. IMS2000, pp. 375-378, June11-16, Boston, MA

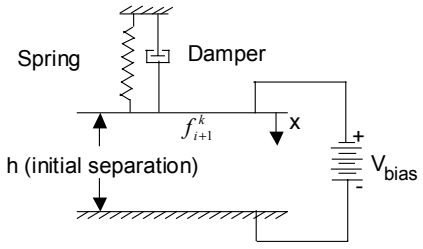

Figure 1: Simplified Capacitor Diagram

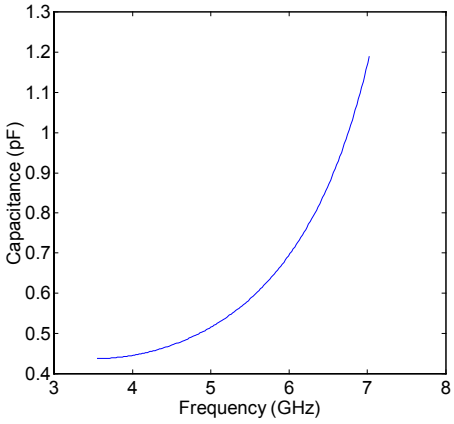

Figure 2: Capacitance vs. frequency for test structure

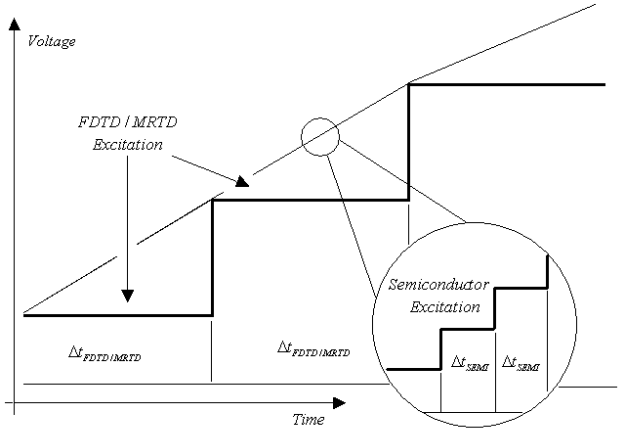

Figure 3: Semiconductor Excitation Interpolation

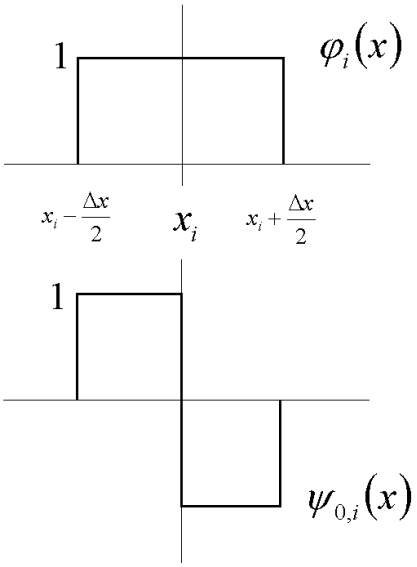

Figure 4: Haar Scaling and Wavelet Functions