Multi-Resolution Time-Domain and Level-Set Techniques for Multi-Domain/Multi-physics/Multi-Phase Simulations

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***Abstract* — In this paper, we present various techniques for the modeling of multi-domain/multi-physics and multi-phase high-frequency problems. The deployment of Multiresolution time-domain principles and of level-set based multi-phase simulation leads to a new generation of computationally efficient tools that could potentially bridge the gap between Maxwell, solid-state and solid/liquid-interface equations. Numerous examples of microelectromechanical, carbon-nanotube and liquid electronics will be presented at the conference verifying the potential of the above approaches.**

***Index Terms* — Multiresolution techniques, wavelets, level-set techniques, multi-physics simulations, biosensors, nanostructures, solid-state, multi-phase structures. Ceramics, coaxial resonators, delay filters, delay-lines, power amplifiers.**

I. INTRODUCTION

The explosive growth in wireless communications (4G Cellular Systems, 60GHz mmW) has spawned a great deal of research in electronic packaging for high performance devices. Silicon-embedded components, flexible ultracompact efficient antennas, integration of micro/nanofluidic channels with multi-phase biological materials and micromachining technology are critical to meet the cost and performance requirements for a higher level of multifunction integration in the development of wireless transceivers, since they can considerably reduce the MMIC real estate and the amount of needed discrete elements. In addition, advances in device processing are enabling the creation of increasingly compact microwave circuits. These advanced devices often utilize geometries with high aspect ratios, small feature size, different phases and moving parts. These characteristics, which are necessary to the operation of these devices, often lead to difficulties in predicting performance. The simulation of these complex devices requires the use of extremely small elements or cells, which can tax many simulation tools beyond their limits. This has led to the use of a combination of methods, such as full-wave simulation and microwave circuit simulation, or, if higher accuracy is required, the use of a parallel full-wave simulator on specialized hardware. For the modeling of all of the above wireless elements, time-domain full-wave techniques demonstrate numerous advantages since they are robust and easy-to-program, they can use wideband excitations that allow for one simulation to cover the entire frequency band of interest and can get easily parallelized on relatively inexpensive hardware making it possible to simulate large structures.

The FDTD method is one of the most mature and versatile time-domain numerical techniques and it has been used for a wide variety of structures. The use of variable gridding along with effective parallelization approaches allows fine details of large structures to be modeled. Curves and diagonal elements can be modeled using stair stepping. In addition, a wide variety of FDTD enhancements make possible the modeling of small gaps, multidielectric/membrane configurations and resonating passives. The MultiResolution Time-Domain Technique (MRTD) [1,2] is an adaptive generalization of the FDTD technique that is based on the principles of Multiresolution analysis and makes use of wavelets to alleviate the computational burdens of FDTD for complex or large structures, such as multilayer packages or MEMS, where the position of the boundaries is time-changing and the membrane thickness is much smaller than any other detail in the transverse direction..The MRTD technique allows the cell resolution to vary with both time and position. The wavelets can be used to represent higher levels of detail along with higher frequency content. As fields propagate through the structure the resolution can be varied to allow for the rapidly changing fields, thus allowing for time- and space-adaptive modeling schemes. The Haar wavelet family is in many ways one of the simplest, however, it has many properties that make its application to practical structures favorable [3], leading to filed expansion such as

$$E_x(x)=\sum_{n,i,j} h_{n(t)}\left[\begin{array}{l} {}_nE^{x,\phi\phi}_{i,j}\varphi_i(x)\varphi_j(y)+ \\ \sum_{r=0}^{r_{\max}}\sum_{p=0}^{2^r-1} {}_nE^{x,\psi\phi}_{i,j,r,p}\psi^r_{i,p}(x)\varphi_j(y)+ \\ \sum_{r=0}^{r_{\max}}\sum_{p=0}^{2^r-1} {}_nE^{x,\phi\psi}_{i,j,r,p}\varphi_i(x)\psi^r_{j,p}(y)+ \\ \sum_{r=0}^{r_{\max}}\sum_{p=0}^{2^r-1}\sum_{s=0}^{r_{\max}}\sum_{q=0}^{2^s-1} {}_nE^{x,\psi\psi}_{i,j,r,p,s,q}\psi^r_{i,p}(x)\psi^s_{j,q}(y) \end{array}\right] \quad (1)$$

In a 2D expansion wavelets and scaling functions are used in both the *x* and *y* directions. The terms in (1) represent the products of the basis functions in both directions. For each of these products, one coefficient results. The four groups of coefficients represent the scaling-*x*/scaling-*y*, wavelet-*x*/scaling-*y*, scaling-*x*/wavelet-*y*, and wavelet-*x*/wavelet-*y* coefficients. There are $2^{2(r_{\max}+1)}$ wavelets for a maximum resolution r_{max}. For a maximum resolution level r_{max}=0, the four coefficients in 2D (one for each product term in (1)) are

978-1-61284-757-3/11/$26.00 C2011 IEEE

presented in Fig. 1. When the E and H field expansions are inserted into Maxwell equations, the method of moments can be applied to determine update equations for each of the wavelet/scaling coefficients [3]. It has been shown [3,4] that the offset $1/2^{r_{max}+2}$ between the E and H fields in this expansion yields the best dispersion properties and locates the equivalent grid points in the same pattern as the FDTD-Yee cell. In the 2D case, like the previously presented 1D case, the equivalent grid points are at the center of the constant valued sections of the highest resolution wavelets. In Fig. 1 these are the locations of the + and – in the $\psi_x\psi_y$ function.

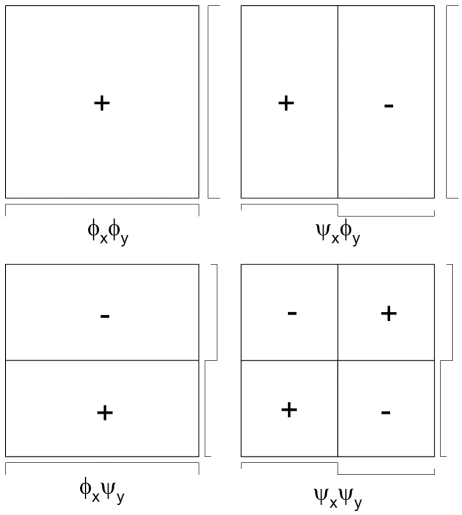

Fig. 1 2D Haar coefficients for r_{max}=0

The update equations for this case are

$$ {}_{n}\mathbf{E}^{x}_{i,j} = {}_{n-1}\mathbf{E}^{x}_{i,j} + \frac{\Delta t}{\varepsilon \Delta y}\left(\mathbf{U}_{E_{x1}\,n-1}\mathbf{H}^{z}_{i,j} + \mathbf{U}_{E_{x2}\,n-1}\mathbf{H}^{z}_{i,j-1}\right) \quad (2) $$

$$ {}_{n}\mathbf{E}^{y}_{i,j} = {}_{n-1}\mathbf{E}^{y}_{i,j} - \frac{\Delta t}{\varepsilon \Delta x}\left(\mathbf{U}_{E_{y1}\,n-1}\mathbf{H}^{z}_{i,j} + \mathbf{U}_{E_{y2}\,n-1}\mathbf{H}^{z}_{i-1,j}\right) \quad (3) $$

$$ {}_{n}\mathbf{H}^{z}_{i,j} = {}_{n-1}\mathbf{H}^{z}_{i,j} + \frac{\Delta t}{\mu}\begin{pmatrix} \frac{1}{\Delta y}\left(\mathbf{U}_{H_{Ex1}\,n-1}\mathbf{E}^{x}_{i,j} + \mathbf{U}_{H_{Ex2}\,n-1}\mathbf{E}^{x}_{i,j+1}\right) \\ -\frac{1}{\Delta x}\left(\mathbf{U}_{H_{Ey1}\,n-1}\mathbf{E}^{y}_{i,j} + \mathbf{U}_{H_{Ey2}\,n-1}\mathbf{E}^{y}_{i+1,j}\right) \end{pmatrix} \quad (4) $$

These equations are written in a matrix form similar to [3], where, for example, each ${}_{n}\mathbf{E}^{x}_{i,j}$ is the vector of the scaling and wavelet coefficients that represent the electric field in the *i,j* cell at time step *n*. The **U** matrices are the results of the inner products from the method of moments and (2)-(4) can be used in a time marching scheme similar to the FDTD method [5]. The resolution can be varied on a cell by cell basis, and can also be changed as a function of time [2].

III. SOLID-STATE STRUCTURES – COUPLING OF MAXWELL'S AND TRANSPORT EQUATIONS

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, velocity v_d, energy w, and electric potential φ:

$$ \frac{\partial n}{\partial t} = \nabla \cdot \left(n\vec{v}_d\right) \quad (5) $$

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

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

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

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. 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 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. This model can benefit from MRTD by including wavelets 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.

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IV. MULTI-PHASE STRUCTURES – COMBINATION OF LIQUID, SOLIDS AND GAS MATERIALS

Lately, there has been a significant effort to build miniaturized biosensors that can monitor the effect of proteins, aminoacids and DNA, while an ever increasing number of 3D RF modules include flexible microfluidic or nanofluidic channels, that commonly carry heat-abducting liquids. In addition, numerous implantable RF devices utilize liquid antennas, while inkjet-printable batteries require the deposition of semi-liquid conductive gels. Plus, many electromechanical-coupled phenomena, such as particle dynamics, cell dynamics electrophoresis and dielectrophoresis are recently being employed for biotechnology and environmental science. Fig.2 shows an example of the level-set function implemented in Matlab for a charged particle or electrode submerged in water. The modeling of the RF performance of these time-varying multi-phase structures requires the development of a new generation of multi-domain/multi-physics numerical simulators. Recently, level set method, proposed by Osher and Sethian [5],[6], has developed to be one of the most successful techniques for the expression of time-varying geometries. The idea of the level set method is to express a boundary in an implicit form, as the zero level set of a high-dimensional function, and then trace the change of the boundary by the deformation of the embedded function; this implicit function both represents nd evolves the boundary.

In a sense, the level set method is a technique to represent moving interfaces or boundaries using a fixed mesh. It is useful for problems where the computational domain is divided into two domains separated by an interface. The interface is represented by a certain level set of isocontour of the level set function, which is a smooth step function that equals zero in a domain and one in the other. The physics interface solves the following equation in order to move the interface with the velocity field **u**

$$\frac{\partial \varphi}{\partial t} + \mathbf{u}\cdot \nabla\varphi = \gamma\nabla\cdot\left(\varepsilon\nabla\varphi - \varphi(1-\varphi)\frac{\nabla\varphi}{|\nabla\varphi|}\right) \quad (6)$$

The terms on the left-hand side give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameter, ε, determines the thickness of the region where ϕ goes smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, ε is constant within each domain and equals the largest value of the mesh size, *h*, within the domain. The parameter γ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If γ is too small, the thickness of the interface might not remain constant, and oscillations in may appear because of numerical instabilities. On the other hand, if γ is too large, the interface moves incorrectly. A suitable value for γ is the maximum magnitude of the velocity field **u**. Before you can solve Eq.(6), it is needed to initialize the level set function such that it varies smoothly from zero to one across the interface by letting ϕ to be zero on one side of the interface and one on the other, denoted as ϕ_o. Then solve

$$\frac{\partial \varphi}{\partial t} = \gamma\nabla\cdot\left(\varepsilon\nabla\varphi - \varphi(1-\varphi)\frac{\nabla\varphi}{|\nabla\varphi|}\right) \quad (7)$$

using ϕ_o as the initial condition from t=0 to t~5ε/γ. The resulting ϕ is smooth across the interface and a suitable initial condition to the level set equation. The unit normal to the interface is given by $\mathbf{n} = \frac{\nabla\varphi}{|\nabla\varphi|}$ (at ϕ=0.5) and the curvature is defined as $k = -\nabla\cdot\mathbf{n}$ (at ϕ=0.5)**.** These variables are available in the physics interface as the *interface normal* and *mean curvature*. The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ. The surface tension force is added to the Navier-Stokes equations as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable. The evolution of the phase field variable is governed by the *Cahn-Hilliard equation*, which is a 4th-order PDE. The Phase Field interface decomposes the Cahn-Hilliard equation into two second-order PDEs. For the level set method, the fluid interface is simply convected with the flow field. The Cahn-Hilliard (C-H) equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The Cahn-Hilliard equation PDE governing the phase field variable is given by:

$$\frac{\partial \varphi}{\partial t} + \mathbf{u}\cdot\nabla\varphi = \nabla\cdot\gamma\nabla G \quad (8)$$

where G is the chemical potential and γ is the mobility, which determines the time scale of the Cahn-Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. The quantity λ is the mixing energy density and ε is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ, through the equation: $\sigma = 2^{1.5}\lambda/(3\varepsilon)$ The C-H equation forces to take a value of 1 or -1 except in a very thin region on the fluid-fluid interface. The Phase Field interface splits Eq.(8) up into two second-order PDEs (9)-(10):

$$\frac{\partial \varphi}{\partial t} + \mathbf{u}\cdot\nabla\varphi = \nabla\cdot\left(\gamma\lambda/\varepsilon\varepsilon\right)\nabla\psi \quad (9)$$

$$\psi = -\nabla\cdot\left(\varepsilon\varepsilon\nabla\varphi\right) + \left(\varphi\varphi - 1\right)\varphi \quad (10)$$

Due to the different time constants of the Maxwell and the Cahn-Hilliard equation, the interface position determined by eqs. (9)-(10) is used to define the boundary conditions for 1,000-10,000 time-steps of the electromagnetic FDTD/MRTD simulations, that eventually define the electromagnetic force that acts as the new initial condition of the C-H equations.

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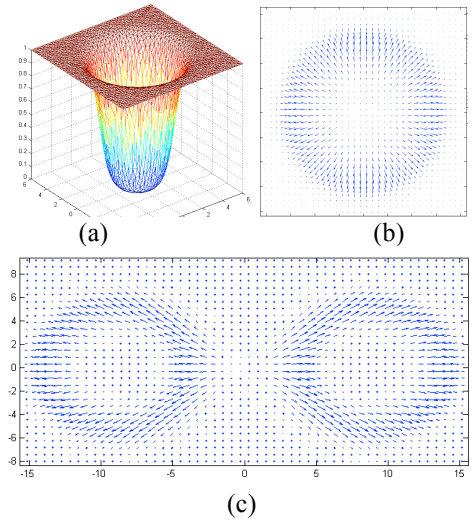

Fig.2 Examples for initializing level-set function in matlab to model a charged object submerged in water (a) Fixed volume charge density of charged object (b) Fixed volume charge gradient of charged object (c) Volume charge gradient of two charged objects of opposite polarity

V. 3D LTCC BENCHMARKING STRUCTURE

A via-fed stacked cavity-backed patch antenna has been designed (based on a 10 layers LTCC process) for the 5.8 GHz WiFi band as shown in Fig. 3. The heights of the lower and upper patches (400 mils × 400 mils) are respectively 8 mils (2 LTCC GL550 layers) and 32 mils.

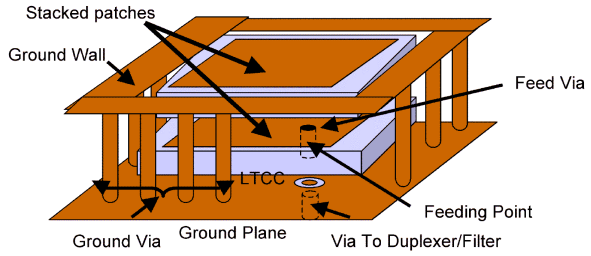

Fig. 3. Double patch cavity batched antenna for 5.725-5.825 GHz applications.

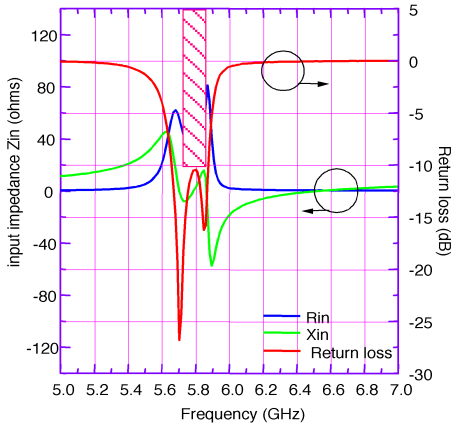

Fig. 4. Input impedance of the stacked patch antenna.

The input impedance characteristic of the stacked-patch antenna is shown in Figure 4. The 10-dB return-loss bandwidth of the antenna is about 4%, fully covering the required band (5.725-5.825 GHz). Conventional FDTD requires a grid of 134x254x266 cells, while MRTD reduced the grid size to 82x132x124. The application of Level-set techniques will be applied to the migration of this design to flexible LCP and results for various curvature radii will be presented at the conference.

VI. CONCLUSION

This paper reviews the application of the multiresolution time-domain (MRTD) and the level-set techniques to the modeling of multi-physics and multi-phase high-frequency topologies.. The time- and space- adaptive grid of MRTD allows it to be used to model finely detailed structures. Areas of the grid containing small features can use increased resolution, while homogenous areas can use low resolution. It is important to note that this technique can be used to model structures with continuous dielectric variations, and thus composite cells, that is those with multiple PEC and dielectric regions per cell, can be modeled. Furthermore, the capability of level-set techniques to accurately represent time-varying phase interfaces can be exploited in the future in the modeling and sensing of liquid/biological substances under the influence of electromagnetic fields as well as in the modeling of flexible inkjet-printed electronics.

VI. ACKNOWLEDGEMENT

We would like to acknowledge IFC/SRC, Microsoft Research Center, NEDO and NSF for supporting this research.

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