Session 1P4
New Challenges and Opportunities in Computational Electromagnetics

A Diagonal Split-cell Model for the High-order Symplectic FDTD Scheme

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Abstract| A high-order symplectic FDTD (SFDTD) scheme using the diagonal split-cell model is presented to analyze electromagnetic scattering of the curved three-dimensional perfectly conducting objects. One the one hand, for the undistorted cells, the fourth-order accurate spatial di®erence is employed. On the other hand, for the completely distorted cells, the treatment of the curved surfaces is based on the diagonal split-cell model. Finally, for the partially distorted cells, the interpolation strategy is proposed to keep the ¯eld components continuous. The numerical experiments suggest that the diagonal SFDTD scheme can obtain more accurate results than both the staircased SFDTD scheme and the traditional diagonal FDTD method. Furthermore, in view of the high numerical stability, the improved symplectic scheme does not need to decrease time increment to comply with the stability criterion.

Multi-physics Simulations of Ion Trap Chemical Sensing

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Abstract| With an increase in importance of applications, chemical sensors are becoming more and more important in homeland security. One of the most powerful sensors is the mass spectrometer, which makes use of the electromagnetic potential well to trap charged molecule (ion) and eject them in the order of their mass charge ratios. These electric ¯eld driven sensors are showing promise for handheld applications. The most traditional ion trap is called Quadrupole Ion Trap (QIT), which is composed of 2 parabolic shaped electrodes with both RF and DC voltages applied to them and has very well described analytical solutions for the electric ¯eld. Many new types of ion traps have evolved, like Circular Ion Trap (CIT) and Rectilinear Ion Trap (RIT) that require numerical electric ¯eld solutions in order to predict performance. Three-dimensional simulations are needed to capture all relevant features of the trap, including injection and ejection slits. In addition, full three-dimensional simulations allow for the simulation of the entire device outside of just the ion trapping region, including the ion optics and sampling interface. Normally the speed of the ion inside the trap can go from 0 to 10^5 m/s in a very short time, so the ion trajectory is very sensitive to the EM ¯eld. Therefore, very accurate EM ¯eld simulation is a critical step for ion trajectory simulation and ion trap design.
In this work, we introduce of the application of common numerical electromagnetic solvers (Ansoft, HFSS), traditionally used for RF and microwave applications, for use in the chemical detection domain. We investigated the ¯eld solutions of RIT with di®erent mesh densities by using 3-D full wave simulation commercial software HFSS. Moving from 2-D to 3-D ion motion simulation, we calculated and compared mass spectrum and accuracy of these solutions. For ion trap simulation, the smoothness of the ¯eld is very important since a discontinuity of the ¯eld will signi¯cantly a®ect the ion motion, while not changing the bulk electrical properties, such as capacitance, port impedance, or energy which are normally used as convergence criteria if the

simulation is used only for the electrical domain. Therefore, we introduce new ¯eld convergence parameters: the smoothness factor *S* and Delta *S*, as convergence criterions which account for the multi-physics application such as ion trapping. By comparing them versus other simulation criterion, we found they can better indicate the smoothness of the solutions, and combined with the traditional delta energy convergence criterion (¢*E*), they can better indicate the accuracy of the simulation results in the sense of the smoothness of the ¯eld. This is in stark contrast to traditional uses for the full wave simulators in which port parameters, such as *S*-parameter convergence, are used as convergence criteria. In these cases, slight discontinuities in the ¯eld solutions, a natural byproduct of the FEM solution, do not signi¯cantly a®ect the properties. In fact, the ¯eld solutions traditionally are the last features of a structure simulation to converge. From the de¯nitions of *S* and Delta *S* and experimental results, we ¯nd they can very good indicate the quality of simulation and be applied to any other ¯eld simulation case.

Parallel Computational Electromagnetic Method, PCEM, for IC Interconnect and Packaging Analysis

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Abstract| As the size of the IC chips keeps shrinking, electromagnetic e®ects inherent in interconnects, clock trees, and packaging are becoming signi¯cantly important. Due to the extreme complexity of these structures, signal integrity analysis based on Maxwell's equations uncovers more salient physical behavior than various simpli¯ed lumped models. Since generally there are no closed-form solutions for wave equations, computational electromagnetic methods (CEM) based on numerical algorithms are pursued for the accurate solutions.

However, CEM for large-scale chip structures has to deal with millions of dicretizations from the mathematical modeling in either sparse or dense linear algebra systems. Hence, numerous fast algorithms, such as pre-corrected FFT, Fast Multipole Algorithms, and QR Decomposition, etc., were developed to accelerate the excessive solving time needed. These algorithms, however, are facing tough challenges in interconnects and packaging analyses due to the ill-conditioned systems that result from shapes that have extreme aspect ratios in complicated practical structures.

In this talk, two general approaches to improve the speed of a CEM simulation will be discussed ¯rst: *soft way* and *hard way*. The soft way is to develop advanced mathematical algorithms while the hard way is to migrate mature algorithms onto super computers for scalable computations. A problem di±cult to handle by the soft way might be easily manipulated through the hard way, and vis versa. Further more, because most modern fast algorithms are based on the \Divide and Conquer" strategy, it is not di±cult for most of them to be parallelized. In other words, a wonderful marriage between fast algorithms and parallel systems is naturally feasible for PCEM, or parallel-CEM.

As an example,a novel hierarchical capacitance extraction approach based on direct boundary integral equation and parallelized on the world's fastest super computer | IBM Blue Gene/L will be shown. This algorithm enforces interactions between conductors in di®erent enclosed regions to go through the surrounding surfaces. It partitions the simulated geometry into small regions. Each region is meshed and analyzed on di®erent nodes to buid the block capacitance matrix, and thus use the power of parallelization. Then cell matrixes are combined based on boundary conditions to create global capacitance matrix. Since direct boundary integral equation is equivalent to the Huygens' Principle, only a homogeneous Green's function is needed even for piecewise constant inhomogeneous structures. Numerical examples will demonstrate the performance of this algorithm and a Blue Gene system.

Based on the aforementioned practice, the power of parallel computational electromagnetics PCEM and IBM Blue Gene will be summarized for the future interconnects and packaging applications.

Application of Numerical Electromagnetics to Power Delivery Design in ULSI

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Abstract| An integral and highly important part in modern day microprocessor design involves the design and analysis of the power grid structure that feeds power to the billions of transistors used in ULSI. With power taking the mainstage in the design °ow it is becoming increasingly important to characterize the electrical performance of these power grids accurately and fast. It has become increasingly evident that incorrect design of the power grid which can allow, over the entire die, even a 10% variation in the voltage can lead to system malfunctions, which ¯nally in°uence the bottomline. To add to this, the decreasing supply voltage has reduced the tolerance for variation in voltage. Lack of accurate models for the power grid has led to increased use of decoupling capacitors in the design which more often than not leads to larger die sizes. This presentation will highlight the reasons that make the fast and accurate modeling of the power delivery design extremely challenging. Past e®orts at addressing this problem will be brie°y explained and we will ¯nally close with the present state of the art.

A Highly E±cient Finite Element Domain Decomposition Method for Analysis of Large-scale Photonic Crystal Problems

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Abstract| Typical photonic crystal problems consist of a large ¯nite array of cylindrical objects embedded in a uniform medium, or more often, a large ¯nite array of cylindrical holes drilled in a uniform medium, arranged in a rectangular or triangular lattice, with some of the unit cells altered to provide certain desired electromagnetic properties. Their analysis requires solving classic Maxwell's equations, and currently such an analysis is mostly carried out using the ¯nite-di®erence time-domain (FDTD) method to gain a basic understanding of physics involved. However, because of the large problem size and also the resonant nature of photonic crystals, the FDTD simulation is very time consuming and thus is ine±cient as a design tool for developing novel photonic crystal devices. In this paper, we propose a new simulation technique for the analysis of large-scale photonic crystal problems. This technique is based on the frequency-domain ¯nite element method (FEM) combined with a highly robust non-overlapping domain decomposition algorithm, which is referred to here as the dual-primal ¯nite element tearing and interconnecting method for electromagnetic analysis (FETI-DPEM). In this method, a ¯nite array is ¯rst decomposed into many subdomains, each of which contains a unit cell. The ¯eld inside each subdomain is formulated using the FEM by solving the vector curl-curl wave equation using curvilinear higher-order vector ¯nite elements. The ¯eld continuity is enforced explicitly along the edges shared by more than two subdomains and implicitly at the interfaces between two subdomains through the use of Lagrange multipliers. The enforcement of the ¯eld continuity couples all the subdomain problems and forms a large global problem, which is composed of decoupled sub-matrices in the block diagonal from each subdomain. With the aid of a direct sparse solver for each subdomain system, the large global problem is reduced to a much smaller interface problem with its size equal to the number of dual unknowns at the interfaces, from which a Neumann boundary condition is obtained at the interfaces between all the subdomains. This Neumann boundary condition is then used to calculate the ¯eld within each subdomain. In this paper, we apply the FETI-DPEM method to the simulation of several photonic crystal problems such as photonic bandgap waveguides and channel drop ¯lters to demonstrate the e±ciency and capability of the FETI-DPEM method.

On High-capacity Computational Electromagnetic Solutions for Future High-speed IC Design

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Abstract|IC design has been guided by circuit theory for more than three decades. As on-chip designers travel deeper and deeper into the submicron regime, computational electromagnetics, the science of solving Maxwell's equations, has increasingly become essential for high-performance IC design. The reasons are three-fold:

² *Reduced feature sizes*. At the 45nm processing technology node and beyond, the IC industry will have to print features that are several times less than the wavelength of light (193 nm) being used. In this regime, light does not propagate in straight lines. Instead, it is a wave. This induces extreme proximity e®ects, which need to be comprehended and compensated for by Optical Proximity Correction (OPC). OPC determines the photomask patterns that enable drawn layout features to be faithfully and accurately reproduced by optical lithography onto the wafer. It has emerged as one of the major gating factors in achieving e±cient turnaround time for IC data preparation and high-yield manufacturing. The enabling technology of accurate model-guided OPC is computational electromagnetics.

² *Increased clock frequency*. Currently the clock frequency of microprocessors is in the gigahertz regime. Since it is necessary to analyze the chip response to harmonics 5 times the clock frequency, it is expected that interconnects would have to be analyzed with certain electromagnetic e®ects incorporated at high frequencies. In 2001, an Intel research team for the ¯rst time quantitatively demonstrated, via simulation and real silicon measurements, the importance of electromagnetic (EM) analysis at tens of GHz [1, 2]. This ¯nding pushes on-chip designers to the verge of the transition from circuit-based design methodology to a ¯eld-based methodology that has full-wave electromagnetic accuracy.

² *Increased Integration of computing and communication*. This calls for increasing levels of the integration of RF, analog, and digital circuits on the same chip, which leads often to undesirable coupling and sometimes to system failure. Prevailing circuit-based signal integrity paradigms are reaching their limits of predictive accuracy when applied to high-frequency mixed-signal settings. To sustain the scaling and integration of digital, analog, mixed-signal, and RF circuitry, a computational electromagnetic solution is indispensable. However, very large-scale IC design (1) demands very large scale electromagnetic solutions, and (2) imposes many unique modeling challenges that are totally new to the electromagnetic community [3]. Therefore it is of paramount importance to develop innovative *high-capacity* computational EM methods amenable for onchip problems so that the VLSI revolution can continue uninterrupted.

In this talk, we will introduce a class of high-capacity computational electromagnetic methods being developed at Purdue University under the support of Intel Corporation.

Applying Equivalence Principle Algorithm in Mixed Scale Electromagnetic Problems

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Abstract| With the successful developments of computational electromagnetic solvers, a variety of large problems can be addressed using computers. Fast EM solvers can solve problems of millions of unknowns from very low to high frequencies. However, still very challenging is the mixed scale problems, such as a tiny object mounted on a large and smooth object, or an electrically large structure constructed by many small elements. These problems often appears in antenna simulation in complex environments, electric circuit performance analysis, etc.. The tiny structures needs to be modeled with a large number of geometrical elements to catch their

features, which results a big number of unknowns and a poorly-conditioned matrix equation that converges slowly when using iterative solvers.
In this talk, an equivalence principle algorithm (EPA) is proposed to ¯x the above problems. Based on the well-known equivalence principle, the low-frequency part of the problem can be decomposed into several domains enclosed by equivalence surfaces (ES) and isolated from the other parts of the objects. The electric and magnetic currents de¯ned on the ES substitute the currents on the inside objects to represent the inside domain. Since the radiation ¯eld of small-size unknowns is smooth, the unknown density on the corresponding ES's can be much less than the one on the objects, which also leads the ¯nal matrix equation away from ill-conditioning. In EPA, translation operators are de¯ned to compute the incident equivalent currents from currents on other ES's or conductors. Equivalence principle operator (EPO), similar to scattering operator, is used to compute the scattered currents from incident currents. The information of the enclosed objects is then embedded in the EPO. Because it can be reused for identical domains, EPA is advantageous in simulating periodic or almost-periodic structures, which reduce the memory usage of EPOs to only the usage of EPO for one domain plus unknowns on the ES. The initial work similarly can be found in [1]. Many other researchers have also investigated this idea [2{6]. The list here is not complete due to the space limitation.
There are many ways to construct EPOs, either direct computation or solving the matrix equation constructed by equivalence principle. The latter one, similarly to the other integral equation formulation, involves only L and K operators. And more equations than needed can be derived from the equivalence principle. A linear combination among them must be selected carefully to remove the internal resonances. While, direct computation of the scattered current is also free of internal resonance.
The challenges in implementing EPA arises when a conductor carrying electric current cut in the middle. The charges accumulated at the cli® will produce singular ¯eld that is hard to model numerically. To avoid this singularity, a tap basis scheme is developed that can keep the current continuity between the inside and outside parts of the object. In the optimization of EPA, contact unknown reduction scheme is applied to reduce the unknown number on the ES. Only one unknown needs to be reserved when two are attached to each other because the tangential continuity of the ¯eld. Moreover, the attached equivalent currents will cancel each other that produce zeros ¯eld to the ES other than their own. The computation of the interaction among unattached unknowns can be accelerated using fast algorithms such as multi-level fast multiple algorithm. With these optimizations, the large mixed-scale problem can be solved e±ciently.

2nd Order ABC in Vector Finite Element Methods for Inhomogeneous Media

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Abstract| The Absorbing Boundary Conditions (ABCs) have been very popular in ¯nite di®erence formulations for modeling electromagnetic wave propagation in unbounded domains, particularly, in the ¯nite di®erence time domain (FDTD) algorithms. To reduce the ¯ctitious re°ections from the truncated boundaries, the usual approach is to incorporate higher order ABCs into the formulation. However, this approach does not enjoy the same degree of success in the vector ¯nite element methods (VFEMs). To date, only 1st order ABC (or impedance boundary condition) is readily and correctly implemented in the VFEMs for modeling unbounded electromagnetic wave propagation. The main di±culty stems from the incompatibility of the functional requirements for the higher order ABCs and the H(curl) conformity of the vector ¯nite elements.
Subsequently, in recent years, most of the VFEM formulations adopt the perfect matched absorber (PMA) method to truncate the in¯nite domain into a ¯nite computational region. The use of the PMA, however, does impose several di±culties: large number of extra degree of freedom, poor condition number in the frequency domain VFEM matrices, and the instability issues

in the time domain VFEM formulations, just to name a few. In this paper, we shall introduce an additional charge variable in the 2nd order ABC formulation, and implement it through the newly developed cement technique. In doing so, the functional spaces of all the variables are now compatible to each other, and the Galerkin nature of the VFEM is then preserved throughout the formulation. We shall show through numerical examples, the proposed 2nd order ABC o®ers distinctive bene¯ts compared to the PMA approach with similar number of unknowns. Moreover, the 2nd order ABC derived is aiming for inhomogeneous media and is then readily applicable to inhomogeneous waveguiding structures, and will be employed as a 2nd order transmission condition in the domain decomposition methods.

Application of Rational Function Approximation Technique to Hybrid FE/BI/MLFMA for 3D Scattering

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Abstract| The rational function approximation technique (RFAT) is applied to the hybrid ¯nite-element/boundary-integral/multilevel fast multipole algorithm (FE/BI/MLFMA) to acquire wide-band and wide-angle backscatter radar-cross-section (RCS) by complex targets in this paper. The two approaches of utilizing the rational function approximation technique, asymptotic waveform evaluation (AWE) and model-based parameter estimation (MBPE), both have been investigated and compared by theoretical analysis and numerical experiments. The numerical results acquired by the developed computing algorithm of integrating the hybrid FE/BI/MLFMA with the RFAT are presented in the paper, demonstrating that the rational function approximation technique can greatly speed up the hybrid FE/BI/MLFMA to acquire wide-band and wide-angle backscatter radar-cross-section (RCS) by complex targets.

A Twofold Iterative Algorithm with Multilevel ILU Preconditioning of Hybrid FE/BI/MLFMA for 3D Scattering

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Abstract| This paper presents a twofold iterative algorithm (TA) with a multilevel incomplete LU (MILU) preconditioning for solving hybrid FE/BI/MLFMA matrix equation for 3D scattering problem. The numerical performance of the proposed algorithm has been compared to the previous decomposition algorithm (DA) as well as conventional algorithm (CA). It is found that the proposed algorithm exhibits superior e±ciency and consumes far less memory. Finally, various numerical experiments have been carried out using the TA with MILU. Numerical results demonstrate that the TA with the MILU o®er a good compromise between robustness and e±ciency, and greatly improve the applicability of the hybrid FE/BI/MLFMA.