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FY06 LDRD Final Report: Broadband Radiation and Scattering

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Broadband Radiation and Scattering
LDRD Project Tracking Code: 01-ERD-005

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Abstract

This is the final report for LDRD 01-ERD-005. The Principle Investigator was Robert Sharpe. Collaborators included Niel Madsen, Benjamin Fasenfest, John D. Rockway, of the Defense Sciences Engineering Division (DSED), Vikram Jandhyala and James Pingenot from the University of Washington, and Mark Stowell of the Center for Applications Development and Software Engineering (CADSE). It should be noted that Benjamin Fasenfest and Mark Stowell were partially supported under other funding.

The purpose of this LDRD effort was to enhance LLNL's computational electromagnetics capability in the area of broadband radiation and scattering. For radiation and scattering problems our transient EM codes are limited by the approximate Radiation Boundary Conditions (RBC's) used to model the radiation into an infinite space. Improved RBC's were researched, developed, and incorporated into the existing EMSolve finite-element code to provide a 10-100x improvement in the accuracy of the boundary conditions. Section I provides an introduction to the project and the project goals. Section II provides a summary of the project's research and accomplishments as presented in the attached papers.

I. Introduction

Time-domain electromagnetics simulations can be split into two categories: those in which the fields are completely contained by a perfect conductor, and those in which the fields radiate into an unbounded space. For contained problems, the accuracy of our EM codes is limited solely by computational resources. The LLNL finite-element code EMSolve [1][2][3] has been demonstrated to be highly accurate for interior-type problems. It is a massively parallel code, and can efficiently make use of very large Linux clusters. However, its accuracy has been limited for unbounded problems by the accuracy of its radiating boundary condition (RBC), which models radiation out of the problem domain. Many EM analysis problems require the modeling of radiation into free space. Problems such as the analysis of electro-optical devices for NIF and broadband antenna and radar simulations are examples of open problems well suited to time-domain simulations.

Before this project, the EMSolve code was capable of delivering qualitatively correct solutions to EM radiation and scattering problems, but it was not possible to achieve arbitrary accuracy. The RBC's were the limiting factor. Two approaches were taken to provide two separate improved RBC's. The first approach was to extend the so-called Perfectly Matched Layer (PML) concept already employed in EMSolve. A PML is essentially a fictitious material designed to absorb the outgoing waves. The PML used is a provably stable uniaxial PML. The PML was extended to be compatible with higher-order spatial and temporal discretization. The extensions followed the research of Ziolkowski [4], Jin [5] and others. The completed PML was incorporated in published conference [6] and paper [7] results.

The second approach was to investigate using a boundary integral formulation for the scattered fields The boundary integral approach relies upon the use an integral equation to predict the value of the **E** and **H** fields on the mesh boundary at time $t = t^n$, given the **E** and **H** fields on the mesh boundary at all previous times t^{n-1}, t^{n-2}, ... The boundary integral formulation used for radiation into open space is coupled with the finite element method for the interior, resulting in a so-called hybrid FEM/BEM method. These hybrid methods have been used quite successfully in frequency domain electromagnetics, such as in the LLNL EIGER code [8].

The integral equation used to compute the **E** and **H** fields on the mesh boundary is not unique. Ziolkowski and Madsen [9] investigated an approach that employed distinct "source" and "observation" surfaces. The method worked, but it was prohibitively expensive on the 1980's computers, and was restricted to a Cartesian grid FDTD. More recent advances [10] have extended this technique to tetrahedral-based FEM solving the vector wave equation. This research effort extended previous work to include hexahedral finite elements for the solution of the coupled first-order Maxwell's equations. In addition, it incorporated numerous stability enhancements to the boundary condition, such as sub-cycling the boundary element segment of the problem [11] and using highly exact polar integration [12].

If n represents the number of field unknowns on the surface, a straightforward implementation of the BEM equation results in an $O(n^2)$ algorithm. For small and medium sized problems the $O(n^2)$ complexity is not a showstopper on modern cluster computers. However, for more routine electromagnetic analyses or design optimizations that may require 100's of simulations this cost difficult to handle. There have been recent advances in fast methods for time-domain boundary integral solutions that are based on plane-wave expansions of the field [10], or projection to an auxiliary regular grid [13]. These techniques can potentially yield $O(n \log n)$ performance. These approaches are complicated and extremely difficult to apply to parallel computing. A multiresolution approach to fast methods was attempted and is presented in [12].

II. Results and Summary of Selected Publications

The perfectly-matched layer (PML) implementation was extended to higher-order elements and higher-order time integration. A uniaxial PML was developed, consisting of an anisotropic material with both magnetic and electric conductivity. A cubic polynomial was used to ramp the conductivity from zero (at the PML/problem interface) to a maximum value at the other edge of the PML. The optimal choice for the maximum value of the electric conductivity in the PML was found to be

$$\sigma_{\max} = \frac{3\varepsilon}{dt},$$

where ε epsilon is the permittivity of the PML region, and dt is the timestep used. For the magnetic conductivity,

$$\sigma^{M}{}_{\max} = \frac{3\mu}{dt},$$

with μ the permeability of the PML region was used. The PML was tested and found to provide reflections as small as –71 dB in a coaxial waveguide. The PML was also used a very large simulation of a photonic band-gap waveguide. These waveguides offer the advantage of low-loss transmission around very sharp 90-degree bends. This simulation, showing the performance of the PML, is described in more detail in [6], attached.

The first step in implementing the hybrid BEM/FEM boundary condition was the development of BEM basis functions that were complementary to those already used in EMSolve. Surface basis functions were developed based on the underlying concept of differential forms used for the basis functions in EMSolve. The basis functions are first formed on a reference element, then transformed onto the real elements of the mesh. This technique allows much of the work in computing the basis function to be reused for every basis function. The basis functions developed provide improved conditioning of the solution matrices when compared to more common RWG [14] basis functions. These basis functions were compared to those in EIGER for several problems, and shown to offer up to a factor of 10^3 improvement in the condition number of the system matrix for frequency domain problems. The basis function transforms and detailed results are presented in [15], attached.

After the basis functions were developed, the next step was to create a stand-alone time-domain BEM code. The primary challenge to developing this code was stability. Many BEM formulations display late-time instabilities when implemented. While many researchers have studied stability, hard rules to guarantee stability have not been generated. During our work, it was found that highly accurate integration as well as selection of a large enough time step was essential for stability. In order to ensure accurate integration of the potentials used in forming the system matrix, a polar integration scheme was developed. While standard quadrature techniques can accurately evaluate the spatial changes in current, the polar technique also accurately captures the temporal variations in current, helping to lower the necessary timestep for stability. This integration technique is presented in section two of [12], attached. Section three of [12] also presents an exploration of a multilevel fast method for the BEM hybrid kernel. The method offered the potential of an *O(n)* algorithm. However, it failed to be accurate in practice.

With a working parallel time-domain BEM code in place, the development of the true hybrid could begin. There are several ways to incorporate the integral equations as a boundary condition for the finite elements. The method that was chosen was that of a two surface hybrid. Equivalent electric and magnetic currents were computed on an inner surface from the electric and magnetic fields calculated by the finite-elements. The integral equation formulation was then used to find the electric and magnetic fields generated by these currents at the outer boundary of the mesh. Several different methods of applying these fields to terminate the finite element mesh were tested. In particular, using the electric field as a Dirichlet boundary condition or the magnetic field as a Neumann boundary condition were tried. However, it was determined that the best results were obtained when using a weighted combination of the two fields. To accelerate the computation of the boundary condition, it was discovered that the boundary element timestep should be chosen to be some multiple of the finite element timestep. This improved late-time instability problems and increased the speed of computing the boundary condition by a factor of two or more.

The hybrid boundary condition was tested on a number of scattering and radiation problems, and was shown to be more accurate than the first order ABC. While the hybrid boundary condition is slow in general, it can be faster than the ABC in some cases. The ABC requires padding the problem out with air to ensure that radiated waves impinge on the boundary at near normal incidence. The hybrid boundary condition has no such restrictions; the boundary can be placed as little as two cells away from the structures of interest. For some problems, the cost of computing the finite-element solution in the extra air regions outweighs the cost of using the more expensive hybrid boundary condition. One example of this is in generating the scattered field returned from the rocket used in [11]. For this particular problem, the hybrid solution required 45 minutes on 16 processors while the ABC took 1 hour and 48 minutes on 64 processors. The details of the hybrid boundary condition as well as numerous results can be found in [11], attached.

III. Conclusions and Summary

Two types of highly accurate radiating boundary conditions, the PML and the hybrid BEM/FEM boundary, were developed and incorporated into the EMSolve time domain finite-element code. The PML was expanded to incorporate higher-order elements and higher-order time stepping for improved accuracy. This boundary was used to simulate several problems, including a photonic band-gap waveguide structure. Three separate formulations were tested for the BEM/FEM hybrid, based on terminating the finite element mesh with the Electric field, Magnetic field, or a combination of both. It was determined that the combination of both fields led to a better solution. The hybrid problem was found to have several orders of magnitude better accuracy then the ABC for a simple antenna problem, and was used on large scattering problems. While a decrease in the computational scaling below $O(n^2)$ for the hybrid boundary condition was not achieved, the use of sub-cycling for the boundary element portion of the computation as well as the reduced sizes of the volume meshes required when using the hybrid formulation make it a competitive choice for many problems when high accuracy is required.

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