Parallel-MLFMA Solutions of Large-Scale Problems Involving Composite Objects

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Abstract—We present a parallel implementation of the multilevel fast multipole algorithm (MLFMA) for fast and accurate solutions of large-scale electromagnetics problems involving composite objects with dielectric and metallic parts. Problems are formulated with the electric and magnetic current combined-field integral equation (JMCFIE) and solved iteratively with MLFMA on distributed-memory architectures. Numerical examples involving canonical and complicated objects, such as optical metamaterials, are presented to demonstrate the accuracy and efficiency of the implementation.

I. INTRODUCTION

In recent years, parallelization of the multilevel fast multipole algorithm (MLFMA) [1] has enabled the solution of extremely large electromagnetics problems discretized with hundreds of millions of unknowns [2]–[6]. On the other hand, most of the previous implementations have been developed for metallic objects and less attention has been paid to dielectric objects, and especially, to more complex structures involving multiple dielectric and metallic parts [2]. Recently, we showed that the hierarchical strategy, which was originally proposed for metallic objects [3],[5], can be applied to homogeneous dielectric objects [6] for efficient parallel simulations. In this work, we further extend the hierarchical strategy to general objects with coexisting multiple dielectric and/or metallic parts. The developed implementation provides fast and accurate solutions of real-life problems, such as metamaterials at optical frequencies, discretized with large numbers of unknowns.

II. PARALLEL IMPLEMENTATION

The parallel implementation consists of the following major components that are summarized briefly.

A. Formulation, Discretization, and Near-Zone Interactions

Problems are formulated with the electric and magnetic current combined-field integral equation (JMCFIE) and discretized with the oriented Rao-Wilton-Glisson (RWG) functions on small planar triangles. Interactions between nearby basis and testing functions are calculated via singularity extraction and adaptive integration techniques.

B. Iterative Solutions and Far-Zone Interactions

For each penetrable region and matrix partition (i.e., $Z_{JJ}$, $Z_{JM}$, $Z_{MJ}$, and $Z_{MM}$), a multilevel tree structure is constructed by placing the associated surfaces (interfaces) in a cubic box and recursively dividing them into subboxes. A region may consist of multiple unconnected subregions (with the same electrical parameters), which are considered together in the same tree structure. Hence, an overall matrix-vector multiplication (required for iterative solutions) is obtained by tracing different tree structures and superposing interactions in different media. Also note that each trace is a sequence of aggregation, translation, and disaggregation stages, as usually defined for MLFMA. Radiated and incoming fields are sampled with the sampling rate determined by the excess bandwidth formula. Interpolations and anterpolations are carried out using the Lagrange method. Iterative solutions are accelerated by the block-diagonal preconditioners.

C. Parallelization

Each tree structure (constructed for each medium and partition) is parallelized using the hierarchical strategy, which is based on the simultaneous partitioning of subboxes and field samples at all levels. Specifically, for each tree structure, partitions of subboxes and their samples can be optimized to improve the load balancing and to minimize communications. Considering two-dimensional partitioning [3], three different types of one-to-one communications are required: Vertical communications during aggregation/disaggregation, horizontal communications during translations, and data exchanges between pairs of processes to modify partitioning. Code rearrangements are performed to improve the memory recycling and to enable the solution of large problems on moderate computers.

III. NUMERICAL RESULTS

Fig. 1 presents the solution of canonical problems involving a spherical object. A dielectric sphere of radius 50 μm (core) is placed inside another dielectric sphere of radius 100 μm (shell) and located in vacuum (host medium). The relative permittivities of the core and shell are 2.0 and 3.0, respectively. The object is illuminated by a plane wave at 48 THz, 96 THz, and 192 THz. At these frequencies, the size of the object corresponds to approximately $16\lambda_0$, $32\lambda_0$, and $64\lambda_0$, respectively, where $\lambda_0$ is the wavelength in the host medium. For numerical solutions, MLFMA is parallelized into 64 processes using the hierarchical strategy on a cluster of Intel Xeon Nehalem quad-core processors with 2.80 GHz clock rate. The
Fig. 1. Solutions of large-scale scattering problems involving a spherical object, which consists of a dielectric core of radius 50 \( \mu \text{m} \) inside a dielectric shell of radius 100 \( \mu \text{m} \), at 48 THz, 96 THz, and 192 THz.

The largest problem (at 192 THz) is discretized with 52,451,328 unknowns and solved in approximately 24 hours. Fig. 1 depicts the bistatic scattering cross section (SCS) values (in dB\( \mu \text{m} \)) as a function of the bistatic angle from 0\( ^\circ \) to 180\( ^\circ \), where 0\( ^\circ \) corresponds to the forward-scattering direction. Computational values agree well with reference values obtained via analytical Mie-series solutions. The root-mean-square (RMS) error in the RCS values is around 1\% at all three frequencies.

Fig. 2 presents the solution of an electromagnetics problem involving a metamaterial designed for optical frequencies. A total of 101\( \times \)101 metallic rods are enclosed in a lossy shell with a complex relative permittivity of 9.6 + 0.4i. Geometries and dimensions of the rods and shell are described in Fig. 2. The structure is illuminated by a plane wave at 417 THz. The problem is discretized with 13,224,714 unknowns and solved by MLFMA (parallelized into 64 processes using the hierarchical strategy on the Intel Xeon cluster) in less than 16 hours. Fig. 2 depicts the total electric field in the vicinity of the structure. Considering only the host medium in accordance with the equivalence principle [6], electromagnetic fields should vanish inside the object. Fig. 2 demonstrates the high accuracy of the solution, since the electric field inside the object is 50 dB lower than the electric field outside the object.

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