Surface Integral Equation Solvers for Large-Scale Conductors, Metamaterials and Plasmonic Nanostructures

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Abstract – Surface integral equation (SIE) approaches for the accurate solution of different problems in computational electromagnetics are addressed. First, an efficient message passing interface (MPI)/OpenMP parallel implementation of the multilevel fast multipole algorithm-fast Fourier transform (MLFMA-FFT) is presented for the solution of large-scale conducting bodies. By combining the high scalability of the fast multipole method-FFT (FMM-FFT) with the high efficiency of MLFMA, challenging problems up to one billion unknowns are solved using a parallel supercomputer. Second, looking for the extension of these rigorous approaches to new demanded areas, the SIE method is successfully applied to the solution of left-handed metamaterials and plasmonic nanostructures. Numerical examples are presented to confirm the validity and versatility of this approach for the accurate resolution of problems in the context of leading-edge nanoscience and nanotechnology applications.

Index Terms ─ Fast multipole methods, metamaterials, method of moments, parallel programming, plasmonics, supercomputing, surface integral equations.

I. INTRODUCTION

The rigorous solution of radiation and scattering problems using surface-integral-equation (SIE) formulations has commanded a great attention in computational electromagnetics for a long time. Integral-equation techniques, such as the method of moments (MoM) [1], provide accurate results when the surfaces of the problem are properly discretized in terms of the wavelength. Usually, the well-known Rao-Wilton-Glisson (RWG) [2] basis functions defined over planar triangles are applied to expand the unknown surface current density.

In the case of electromagnetic problems involving large-scale conducting bodies, the fast multipole method (FMM) [3] and its multilevel version, the multilevel fast multipole algorithm (MLFMA) [4, 5], are commonly applied in the framework of the iterative solution of the MoM matrix system. The development of these fast (low computational cost) algorithms has gone hand in hand with the constant advances in computer science and technology.

Because of this simultaneous growth, the new methods must be not only fast, efficient and with low complexity, but they also must be able to benefit from the computational capabilities of current high performance computing (HPC) computers and supercomputers. As a consequence, a great attention was focused on the parallelization of MLFMA over shared, distributed, and mixed memory computers. Important advances were achieved in this regard; see among others [6-14].

Another numerical technique that has gained interest in recent years, due to its natural high scalability propensity, is the FMM-fast Fourier transform (FMM-FFT) [15-17]. Using hybrid message passing interface (MPI)/OpenMP parallel implementations of this algorithm and other

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proposed variants (such as nested FMM-FFT and MLFMA-FFT), the authors have demonstrated that this approach constitutes a good alternative to benefit from massively parallel distributed computers, achieving the solution of problems with more than 150, 620, and 1000 million unknowns [17-19].

Up to now, we have been able to analyze very large electromagnetic problems in high-frequency ranges, even reaching the terahertz (THz) region [19]. But growing up in frequency is not only a matter of increasing the number of unknowns. We must reformulate our codes in order to be able to extend their scope of application to emerging fields and areas, such as nanoscience and nanotechnology. In this context, the research in the optical plasmonic properties of metallic nanoparticles and artificial materials (metamaterials) has generated an increasing interest, due to their ability to route and manipulate light at nanometer length scale surpassing the classical diffraction limit.

The optical response of metals is quite different from the metallic conductivity observed at low frequencies. At optical frequencies the penetration of fields can no longer be neglected and the plasmonic optical properties of metals make it impossible to directly downscale the radio-frequency and microwave solutions. Otherwise, by properly engineering the underlying subunits, metamaterials can exhibit exotic optical properties that are not attainable in naturally occurring materials, such as prominent magnetic response or negative index of refraction. To date, the most common way to rigorously accomplish the resolution of such problems has been the use of differential-equation formulations.

Although not yet widespread in optics, the MoM integral-equation approach could bring important advantages for the analysis of homogeneous or piecewise homogeneous plasmonic and/or metamaterial bodies. According to this research interest, our recent efforts were headed to extend the SIE-MoM approach to the analysis of composite piecewise homogeneous metamaterial and plasmonic objects. So, in [20], we successfully applied this formulation to the solution of homogenized left-handed metamaterials. More recently, we generalized this approach to the simulation of arbitrary configurations of composite plasmonic nanoparticles in [21]. From these previous works, it is clear that the SIE-MoM approach can yield very efficient and highly accurate representations of these new electromagnetic problems, taking into account all the physical constraints as determined by the shape and the complex dielectric constants of the particles.

In this paper, we first make a review of the latter method we have proposed for the electromagnetic analysis of large-scale conducting bodies using the SIE formulation, namely, MLFMA-FFT. Then, we focus on the works we are doing presently to extend these techniques to the analysis of non-conventional (generalized) media, such as the left-handed metamaterials and plasmonic nanoparticles at optical frequencies.

II. MLFMA-FFT FOR THE ANALYSIS OF LARGE-SCALE CONDUCTING BODIES

The aim of MLFMA-FFT is to combine the best of MLFMA and FMM-FFT to obtain a highly scalable method with low computational cost, which is suitable to take advantage of existing HPC computers. Initially, the algorithm requires a multilevel octree decomposition of the geometry. The far-field interactions are obtained at the coarsest level of the geometry partition using a global distributed FMM-FFT algorithm [18]. A parallelization strategy based on the distribution of fields, by distributing the *k*-space samples among nodes, has been considered for this stage. Regarding the near-field contributions, they are obtained at the finer levels of the octree by using one or more local executions of MLFMA defined inside each shared-memory computing node.

For the parallel implementation, we have selected a hybrid parallel programming combining MPI with the OpenMP standard, which fits perfectly with mixed-memory computer systems. Thus, the parallel MLFMA-FFT approach provides a significant reduction of the computational complexity while maintaining a high scalability behavior for the solution of extremely large problems using supercomputers.

The main difference of MLFMA-FFT with regard to the original FMM-FFT algorithm is given by the procedure used for dealing with the near couplings. In the MLFMA-FFT method, this task is performed by MLFMA. The partition of work is based on a distribution by octree groups at the coarsest level. This distribution is propagated downward to the finest level. The partial near contributions to the matrix-vector product (MVP) are then computed by several MLFMAs defined over the finer levels (from the finest to one before the coarsest) operating strictly inside each shared-memory computing node. In this way, MLFMA is never distributed among nodes, but it is only applied in shared-memory computations (so it does not suffer from poor parallel scaling).

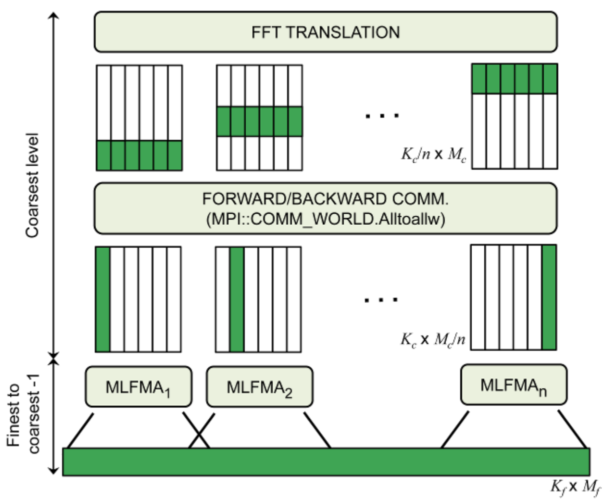

Fig. 1. MLFMA-FFT parallel algorithm.

Figure 1 illustrates the parallel operation of MLFMA-FFT. Let us define parameters K, N, M, and n as the number of k-space samples, the total number of unknowns of the problem, the number of non-empty groups, and the number of nodes, respectively. The subscripts c and f are added to indicate the coarsest and finest levels, respectively. It can be observed in the figure that MLFMA work in levels comprised between the finest and the preceding to the coarsest one. The near coupling contributions to the MVP at the coarsest level are computed at the finer levels by MLFMA inside each node. After the required interpolation of the outcoming fields to the coarsest level, each node has the complete set of directions, K_c, for its assigned M_c/n observation groups. At this point, an all-to-all communication is performed in order to obtain the partial K_c/n samples assigned to each node for all the M_c groups at the coarsest level. This switches from the group-driven distribution to the field-driven distribution.

The required inter-node communications are efficiently carried out during the MVP in a single step by using the asymmetric *MPI::Alltoallw* operation. The *Alltoallw* high-level command makes possible to carry out all the required communications without latency periods or explicit synchronization because of the efficient management provided by the MPI library (we are using the 2.3 version of HP-MPI).

When the 3D-FFT translation is done, the complementary all-to-all communication allows switching back to the group-driven distribution at the lower levels. After that, each node will have the complete K_c directions of the incoming fields for its M_c/n assigned observation boxes at the coarsest level. Starting from this level, these fields are recursively anterpolated, shifted, and combined at the centers of their child groups at the next lower level. Then, the collected incoming pattern of every observation group at the finest level is shifted and evaluated at each belonging testing function, hence providing the far contribution to the MVP for the set of M_c/n observation groups assigned to that node. As for the aggregation and interpolation stage, all the computations are efficiently performed inside each node without inter-node communications.

A. Numerical example

The NASA Almond is analyzed at a frequency of 3 THz with our parallel implementation of the MLFMA-FFT algorithm.

The electric-field integral equation (EFIE), the RWG basis functions, and the Galerkin testing procedure are used. No preconditioning is applied. An incident plane with horizontal polarization wave impinging on the back side of the Almond target is considered, as shown in the inset of Fig. 2. The analysis was done in the *Finis Terrae* supercomputer, consisting of 142 cc-NUMA HP Integrity rx7640 with 8 dual core Intel Itanium2 Montvale processors at 1.6 GHz with 18 MB L3 cache and 128 GB of memory each one. The nodes are interconnected through a high efficiency Infiniband network (4xDDR), and the operating system is Linux SLES 10. The solution of the 1,042,977,546 unknowns matrix system required the use of 64 nodes (involving a total of 1,024 processors) and 5 TB of memory. The setup time was about 105 minutes, while the iterative solution took less than 33 hours to attain a residual error of 0.023 (a total of 8 external GMRES iterations with restart 80 were required). The bistatic radar cross section (RCS) of the Almond is shown in Fig. 2.

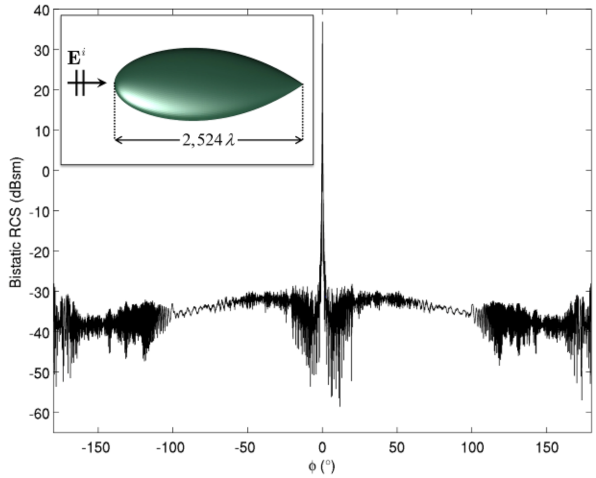

Fig. 2. Bistatic RCS of the NASA Almond target at a frequency of 3 THz.

III. SIE-MoM FOR LEFT-HANDED PLASMONIC MEDIA

When dealing with homogeneous dielectric materials, it is usual to consider the combination of normal (N-EFIE, N-MFIE) and tangential (T-EFIE, T-MFIE) equations derived from the boundary conditions imposed separately to the electric and magnetic fields. Among the multiple possibilities of combination, the following one is proven to be a stable proposal [22, 23]:

$$\begin{aligned}&\sum_{l=1}^{2} a_l \frac{1}{\eta_l}\text{T-EFIE}_l + \sum_{l=1}^{2} b_l \text{N-MFIE}_l \\ &-\sum_{l=1}^{2} c_l \text{N-EFIE}_l + \sum_{l=1}^{2} d_l \eta_l \text{T-MFIE}_l .\end{aligned} \tag{1}$$

In equation (1), η_l is the intrinsic impedance in medium R_1 (R_1 and R_2 are the exterior and interior regions of the material, respectively). Different known formulations can be obtained depending on the selection of the complex combination parameters a_l, b_l, c_l and d_l, as shown in Table 1.

To extend the MoM formulation to the solution of piecewise homogeneous metamaterial and plasmonic penetrable objects we have opted to use the same formulation. Concretely, we concerned ourselves with the formulations known as Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) [24], combined tangential formulation (CTF) and combined normal formulation (CNF) [22], and the electric and magnetic current combined field integral equation (JMCFIE) [25]. PMCHWT and CTF combine tangential equations, CNF combines normal equations, while JMCFIE is the more general formulation combining both tangential and normal equations. For the discretization of the surface electric and magnetic currents, we opted again to use the RWG basis functions, as in the case of perfectly conducting bodies. Accurate calculation of the integrals involved in the evaluation of expressions in (1) using the RWG functions is crucial for the precision of the method. We have applied Gaussian quadrature rules for the numerical integration of smooth varying integrands, together with the analytical extraction procedures of [26-28] for the accurate evaluation of singular integrals.

Table 1: Combining parameters for different penetrable media formulations

Formulation	a_l	b_l	c_l	d_l
PMCHWT	η_l	0	0	$1/\eta_l$
CTF	1	0	0	1
CNF	0	1	1	0
JMCFIE	1	1	1	1

On the other hand, for the application of the above described formulation to the analysis of left-handed materials (LHM) and plasmonic nanoparticles, special care must be taken with the definition of the electromagnetic parameters and properties of the material. Concretely, if region defines a penetrable homogenized left LHM or a plasmonic particle, the following definitions should be applied for the wavenumber and the intrinsic impedance:

$$k_l = \omega\sqrt{\mu_l}\sqrt{\varepsilon_l}, \tag{2}$$

$$\eta_l = \frac{\sqrt{\mu_l}}{\sqrt{\varepsilon_l}}. \tag{3}$$

A. Numerical examples

We include in this section some examples to provide a verification of the validity and efficiency of the SIE-MoM approach for the solution of LHM and plasmonic nanostructures. All of them have been solved by matrix factorization. The first one consists of the simulation of the Snell law experiment for a LHM to demonstrate the negative angle of refraction. A three-dimensional (3-D) prism was considered being $10\lambda_0$ high, $10\lambda_0$ wide, and $4\lambda_0$ deep in the largest dimension, with λ_0 the wavelength of the surrounding free-space medium. The prism is made of LHM with $\varepsilon_r = -1$ and $\mu_r = -1$ (so it is impedance matched to the surrounding space.) The angle of the second surface is 8º. An almost flat Gaussian beam, with a total angular spread of 25º and the waist at a distance of $5\lambda_0$ away is orthogonally impinging onto the first surface of the prism from the right hand side. The incident electric field is horizontally polarized.

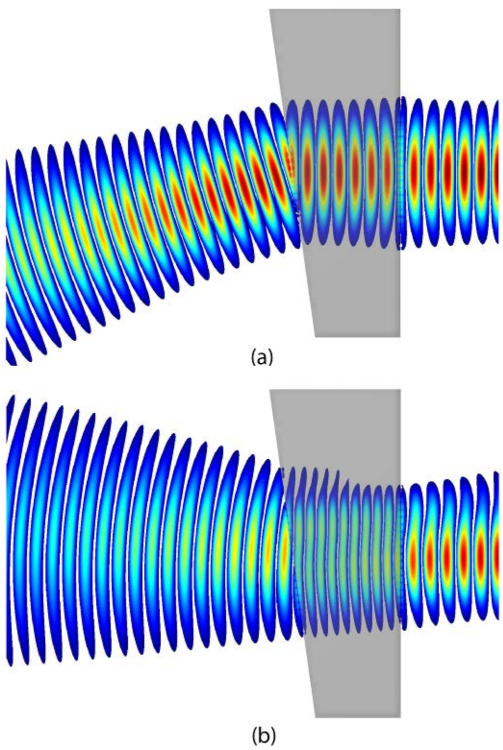

Fig. 3. (a) Incident flat Gaussian beam negatively refracted by impedance matched 3D LHM prism. (b) Conventional refraction from a prism made of Teflon.

Figure 3 (a) shows the computed electric field intensity for the experiment described above considering a refraction index of n = -1 for the LHM comprised prism. The problem was solved with the JMCFIE SIE-MoM formulation using 40,770 unknowns for the equivalent electric and magnetic currents induced on the surfaces of the prism. For the sake of comparison, Fig. 3 (b) shows the same above experiment repeated for a prism made up of conventional material (we have considered Teflon, with ε_r = 2.2). In this case, the refraction is obtained in the conventional direction.

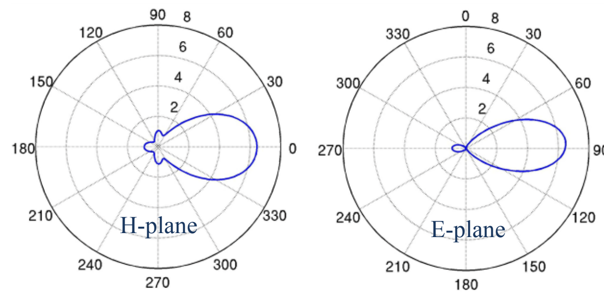

Fig. 4. Directivity of the Yagi-Uda antenna of [30] in dBi for a near-field coupled Hertzian dipole emitter: (left) H-plane ; (right) E-plane.

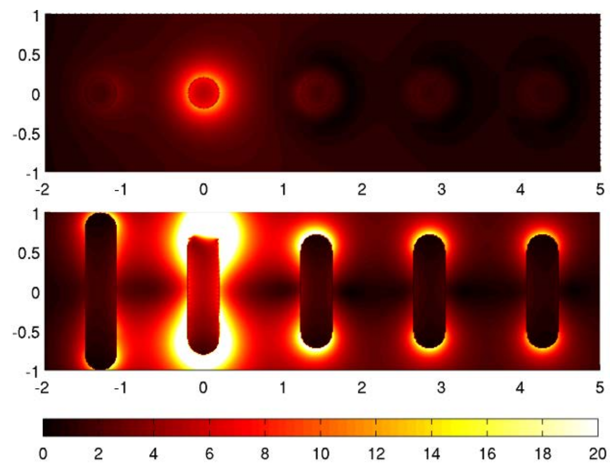

Fig. 5. Near-electric-field (V/m) distribution in the vertical and horizontal planes crossing the Yagi-Uda antenna. Dimensions are in hundreds of nanometers.

A thorough comparison of the accuracy of the usual formulations for problems involving LHMs was presented by the authors in [29].

In order to show the applicability of the method for general 3-D plasmonic nanostructures, the Yagi-Uda optical antenna designed in [30] has been analyzed with the JMCFIE SIE-MoM formulation. The antenna consists of five cylindrical elements made of aluminum, with radius 20 nm and terminated with hemispherical ends. It was optimized for an operating wavelength of λ_0 = 570 nm (in which the relative permittivity constant of aluminum is $\varepsilon_r = -38-10.9j$ and the relative permeability is μ_r = 1). See [20] and [30] for further details of the geometry. The antenna was analyzed using a total of 9,036 basis functions to represent the equivalent electric and magnetic currents on the surfaces of the nanodipoles. The computed directivity in the H- and E-planes for a near-field coupled Hertzian dipole emitter is depicted in Fig. 4. An excellent agreement with the results of [30] can be observed. Finally, Fig. 5 shows the near-electric-field distribution in the vertical and horizontal planes crossing the antenna for the Hertzian dipole excitation.

IV. CONCLUSION

In this work, we present some rigorous integral-equation solutions for different electromagnetic problems. In the case of large-scale metallic bodies, an efficient MPI/OpenMP parallel implementation of the MLFMA-FFT algorithm was shown to combine a low computational cost with a high scalability behavior, which make it an optimal choice to benefit from modern HPC computers and supercomputers. The MLFMA-FFT algorithm exploits the high scalability of FMM-FFT for the distributed computations, while the very efficient MLFMA is applied to expedite the local shared-memory computations. Since MLFMA is not distributed among nodes, but it is locally applied, it does not suffer from poor parallel scaling. In this way, we can say that the best of MLFMA and FMM-FFT algorithms is put together in MLFMA-FFT.

On the other hand, currently our work is headed to extend these rigorous integral-equation techniques to the electromagnetic simulation of problems involving homogenized left-handed metamaterials and plasmonic nanoparticles in the visible or near visible regimes. Different well-known SIE-MoM formulations, usually applied for dielectric bodies, where successfully applied to this kind of media. Numerical examples using the JMCFIE formulation were presented that confirm the validity and versatility of the integral-equation approach to the resolution of LHM and plasmonic problems in the context of leading-edge nanoscience and nanotechnology applications. Besides, it must be noticed that the application of MoM will bring the possibility of applying the latest breakthrough developments in fast integral-equation methods, such as MLFMA-FFT, for the solution of large-scale problems in metamaterials and plasmonics, which will be of great interest for the scientific community.

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The computational challenges analyzed in this paper have been awarded with two international prizes: the PRACE Award 2009, and the Itanium Innovation Alliance Award 2009 in computationally intensive applications.

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