Accuracy: The Frequently Overlooked Parameter in the Solution of Extremely Large Problems

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Abstract—**We investigate error sources and their effects on the accuracy of solutions of extremely large electromagnetics problems with parallel implementations of the multilevel fast multipole algorithm (MLFMA). Accuracy parameters and their effects on the accuracy of MLFMA solutions are studied for large-scale problems discretized with hundreds of millions of unknowns. We show that some error sources are more dominant and should be suppressed for more accurate solutions; identifying less-effective error sources may allow us to derive more efficient implementations. Based on our analysis, we determine a set of benchmark problems that can be used to compare the accuracy of solvers for large-scale computations. A benchmarking tool is provided at `www.cem.bilkent.edu.tr/benchmark`.**

I. Introduction

Recent developments in computational electromagnetics have enabled the solution of many real-life problems with unprecedented levels of size and detail [1]–[10]. Large-scale problems discretized with millions of unknowns can now be investigated easily by sophisticated implementations of efficient algorithms, particularly the multilevel fast multipole algorithm (MLFMA) [1], on state-of-the-art parallel computers [2]–[7],[9],[10]. For example, in the last decade, the number of unknowns that can be solved by MLFMA has increased from tens of millions to more than 1 billion. However, recent studies have focused mainly on the number of unknowns, and less attention has been paid to the accuracy of the solutions. Theoretically, MLFMA is a full-wave solver with controllable accuracy. However, the actual accuracy of a solution and its dependence on various error sources of the algorithm are not obvious. Therefore, for a given problem, its discretization (e.g., the number of unknowns) and the accuracy parameters are not sufficient to assess the accuracy of the solution. This uncertainty of the accuracy also makes it difficult to rigorously compare different implementations, since the solutions may have different accuracies and direct comparisons between the implementations can be unfair.

The aim of this study is to investigate the error sources and their effects on the accuracy of the solutions with MLFMA. Similar studies have been done for relatively small objects, however, accuracy parameters and their roles on the accuracy of the solutions have not been studied for very large problems discretized with hundreds of millions of unknowns. We present accuracy analysis based on comparisons for such very large problems involving both canonical and complicated objects. Investigation of the results leads to new aspects for the optimization of the parallel implementations by suppressing the dominant error sources and relaxing the other parameters towards more efficient solutions. In addition, based on our analysis, we determine a set of benchmark problems that can be used to compare the most recent implementations for large-scale computations.

II. Error Sources

MLFMA implementations involve various error sources that can be categorized as follows:

- Discretization of surfaces using small elements, e.g., planar triangles, with respect to wavelength.
- Discretization of integral-equation formulations using a set of basis and testing functions.
- Direct calculation of near-field interactions using numerical integration methods, e.g., Gaussian quadratures and adaptive techniques.
- Factorization and diagonalization of far-field interactions, e.g., truncation, clustering scheme, and translation strategies.
- Multilevel aggregation and disaggregation, e.g., interpolation and anterpolation techniques.
- Iterative solution, e.g., convergence to the target residual error.

All these error sources are important and affect the accuracy of the solutions, but some of them may dominate the others depending on the problem and the implementation.

III. Numerical Examples

As numerical examples, we consider solutions of a scattering problem involving a sphere of radius 96λ, where λ is the wavelength. The sphere is located at the origin and illuminated by a plane wave propagating in the $-x$ direction with the electric field polarized in the y direction. The problem is formulated with the combined-field integral equation (CFIE) obtained from a linear combination of the electric-field integral equation (EFIE) and the magnetic-field integral equation (MFIE), i.e., $\text{CFIE} = \alpha\text{EFIE} + (1-\alpha)\text{MFIE}$. In
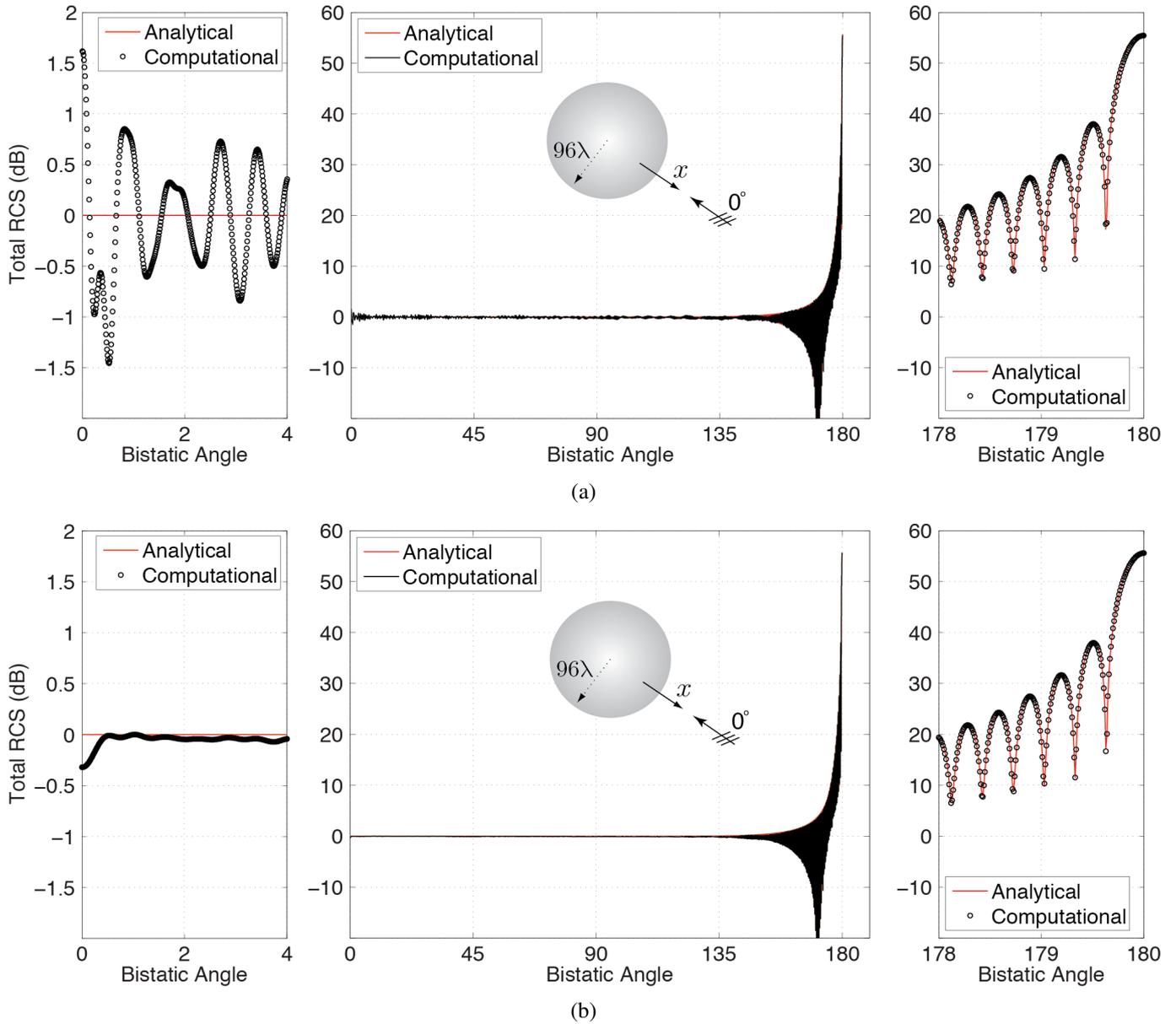
Fig. 1. Solutions of a scattering problem involving a conducting sphere of radius 96λ formulated with CFIE using (a) $\alpha = 0.2$ and (b) $\alpha = 0.6$ discretized with 33,791,232 unknowns.

order to demonstrate the effect of the combination factor α on the accuracy, we consider two different solutions, with $\alpha = 0.2$ and $\alpha = 0.6$. Simultaneous discretizations of surfaces and CFIE formulations using the Rao-Wilton-Glisson (RWG) functions on $\lambda/10$ triangles lead to 33,791,232×33,791,232 dense matrix equations. Near-field interactions are computed with maximum 0.5% error using adaptive integration methods. Far-field interactions are computed with two digits of accuracy using a set of truncation numbers determined by the excess bandwidth formula for the one-box buffer scheme and the worst-case scenario. On the 10-level tree structure involving 0.175λ smallest boxes, interpolations and anterpolations are carried out via a local Lagrange interpolation method with 6×6 stencils. Iterative solutions are performed by the biconjugate-

gradient-stabilized (BiCGStab) algorithm accelerated with a parallel MLFMA [7] and a block-diagonal preconditioner. Convergence to 0.001 residual error is achieved in 20 and 66 iterations for $\alpha = 0.2$ and $\alpha = 0.6$, respectively.

Fig. 1 presents the total bistatic radar cross section (RCS) of the sphere of radius 96λ. The normalized RCS in decibels (dB) is plotted on the x-y plane as a function of the bistatic angle ϕ from $0°$ to $180°$, where $0°$ and $180°$ correspond to the back-scattering and forward-scattering directions, respectively. RCS results around the back-scattering and forward-scattering directions are particularly focused in separate plots. We observe that, in general, computational results agree well with the analytical results obtained by a Mie-series solution. However, one can find different levels of error in a detailed
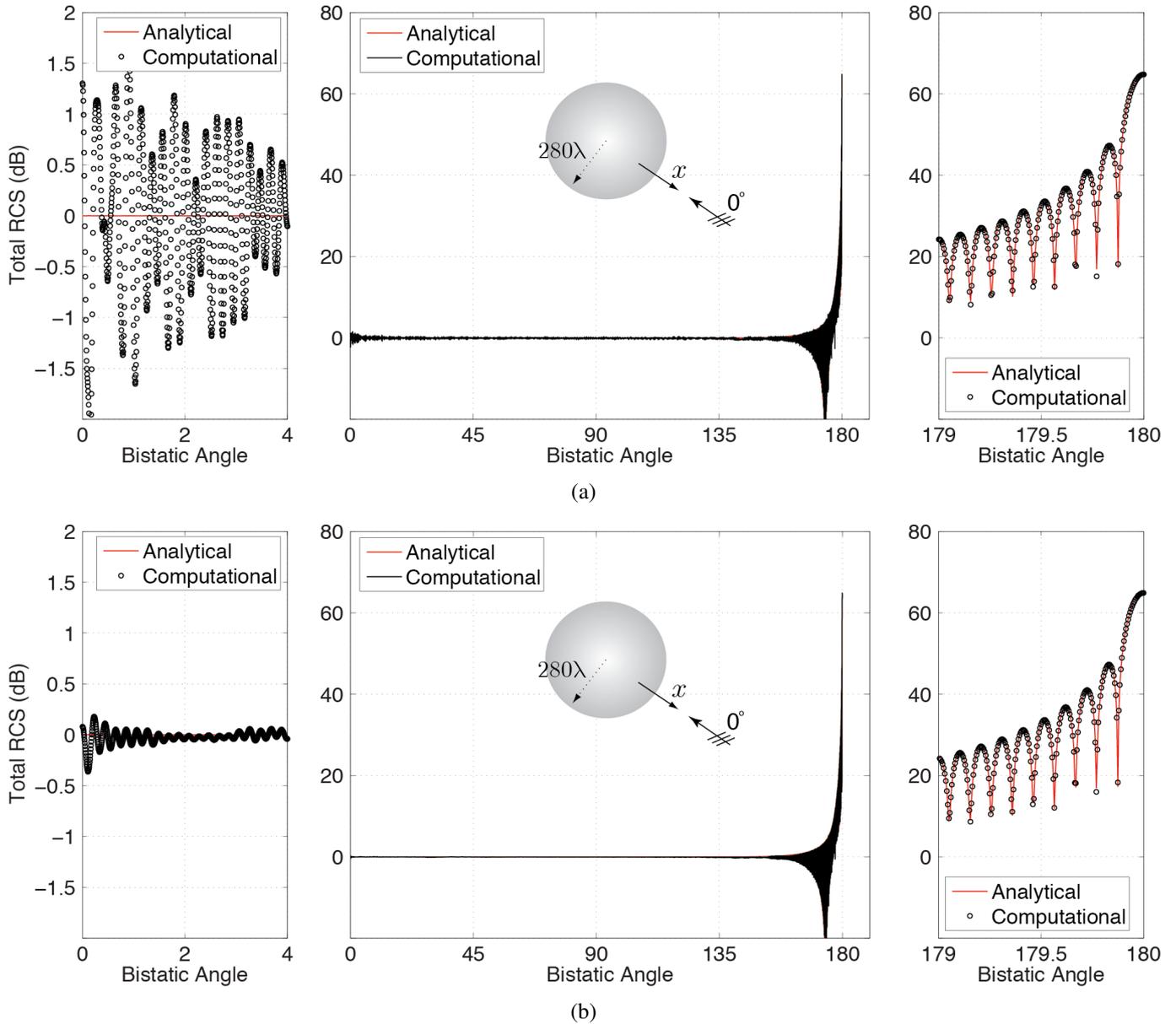
Fig. 2. Solutions of a scattering problem involving a conducting sphere of radius 280λ formulated with CFIE using (a) $\alpha = 0.2$ and (b) $\alpha = 0.6$ discretized with 374,490,624 unknowns.

analysis, such as the focused plot around the back-scattering direction. Specifically, the error is more significant in Fig. 1(a), i.e., when $\alpha = 0.2$ and the MFIE contribution is large in the CFIE formulation. For a more quantitative analysis, we define the relative error in a computational solution with respect to the corresponding analytical solution as

$$\epsilon = \frac{\|\mathrm{RCS}_a - \mathrm{RCS}_c\|_2}{\|\mathrm{RCS}_a\|_2}, \quad (1)$$

where $\| \cdot \|$ represents the 2-norm, and RCS_a and RCS_c are vectors of 1801 elements containing analytical and computational RCS values sampled at $0.1°$ intervals from $\phi = 0°$ to $180°$. For the results depicted in Fig. 1, the relative error is found to be 2.41% and 0.69% when $\alpha = 0.2$ and $\alpha = 0.6$,

respectively. These values clearly show that the combination factor α of CFIE is an important parameter for the accuracy.

Fig. 2 presents solutions of a scattering problem involving a sphere of radius 280λ. The solution parameters are the same as those for the problem depicted in Fig. 1. Discretizations with $\lambda/10$ triangles lead to matrix equations involving 374,490,624 unknowns. As depicted in Fig. 2, the accuracy of the solution is significantly affected by the choice of the combination factor α of CFIE. Specifically, for this problem, the relative error defined in (1) is 1.95% and 0.58% when $\alpha = 0.2$ and $\alpha = 0.6$, respectively. The number of BiCGStab iterations to reduce the residual error to below 10^{-3} increases from 31 to 89 when α changes from 0.2 to 0.6; but we consider this increase in the iteration counts (hence the computing time) acceptable

α of CFIE = 0.2				
Accurate Digits (MLFMA)	0	1	2	3
Relative Error (RCS)	3.96%	2.52%	2.41%	2.38%
α of CFIE = 0.6				
Accurate Digits (MLFMA)	0	1	2	3
Relative Error (RCS)	2.95%	0.74%	0.69%	0.66%

because of the significantly improved accuracy.

Finally, Table I lists the relative error in various solutions of the scattering problem involving the sphere of radius 96λ. For both $\alpha = 0.2$ and $\alpha = 0.6$, we investigate how the accuracy of the far-field interactions (calculated via MLFMA) affects the accuracy of the final result (RCS values). Specifically, the far-field interactions are calculated with zero, one, two, and three digits of accuracy. These values correspond to 100%, 10%, 1%, and 0.1% errors in the worst-case scenario. The following observations can be made:

1) When $\alpha = 0.2$, the number of accurate digits in the far-field interactions has a negligible effect on the final result. For those solutions, the error due to the low-order discretization of the identity operator (in the MFIE contribution) dominates the error arising during the calculation of the far-field interactions.

2) When $\alpha = 0.6$, the discretization error due to the identity operator is moderately suppressed. Hence, calculating the far-field interactions accurately becomes more critical compared to the $\alpha = 0.2$ case. On the other hand, the accuracy is slightly improved when the far-field interactions are calculated with two or three digits of accuracy instead of one digit of accuracy. In other words, there is no need to calculate the far-field interactions with high accuracy (requiring high computational requirements) unless the excessive discretization error is further suppressed. In these solutions, we also note that the near-field interactions are calculated with maximum 0.5% error. Hence, achieving 0.1% error (three digits of accuracy) in the final results may not be possible, even when EFIE ($\alpha = 1.0$) is used instead of CFIE and the far-field interactions are computed with three digits of accuracy.

Surprisingly, numerical examples show that the RCS values obtained with the 0.6 CFIE parameter (and only one digit of accuracy in the far-field interactions) are more accurate than those obtained with the 0.2 CFIE parameter (and three digits of accuracy in the far-field interactions) even though the far-field interactions are calculated 100 times more accurately in the latter.

IV. CONCLUSION

Increasing the problem size and the number of unknowns—a recent trend in computational electromagnetics—should be supported and accompanied by an investigation of the accuracy of the results. An analysis based on the comparisons shows that some of the error sources are more dominant and thus should be suppressed for more accurate solutions. At the same time, identifying less-effective error sources may allow us to derive more efficient implementations by systematically relaxing the corresponding parameters.

Since the solutions obtained from different implementations may have different levels of accuracy, direct comparisons between those implementations in terms of the processing time, parallelization efficiency, and/or memory usage can be unfair. For example, in the literature, it is not uncommon to relax the solution parameters arbitrarily to "increase" the efficiency of the implementation. Therefore, in order to encourage fair comparisons, we determine a set of benchmark problems involving perfectly-conducting canonical objects, such as the sphere and the NASA Almond. Reference solutions are made available on an interactive website at www.cem.bilkent.edu.tr/benchmark to evaluate the accuracy and efficiency of fast solvers.

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