Using Multiple-precision Arithmetic to Prevent Low-frequency Breakdowns in the Diagonalization of the Green's Function

Ö. Ergül and B. Karaosmanoğlu
Department of Electrical and Electronics Engineering
Middle East Technical University, Ankara, Turkey

Abstract— Multiple-precision arithmetic (MPA) is used to prevent low-frequency breakdowns in the diagonalization of the Green's function that is required to implement the multilevel fast multipole algorithm (MLFMA). The breakdown problem is considered at a numerical level, where rounding errors are reduced by increasing the precision as much as required. Using MPA seems to provide a direct solution to low-frequency breakdowns of the standard diagonalization, which may lead to straightforward implementations of broadband MLFMA.

1. INTRODUCTION

The multilevel fast multipole algorithm (MLFMA) is a powerful method for the solution of electromagnetic problems discretized with large numbers of unknowns [1–4]. However, conventional implementations of MLFMA are not efficient for low-frequency problems, where dense discretizations with respect to wavelength are used locally or globally on structures. Specifically, box sizes in MLFMA cannot be very small with respect to wavelength [5], and solutions of such problems involving dense discretizations lead to many interactions that must be calculated directly. It is well known that the diagonalization of the Green's function, i.e., expansion of spherical waves in terms of plane waves [6, 7], is responsible for low-frequency breakdowns. Therefore, in the literature, alternative implementations of MLFMA, such as using explicitly multipoles [8–12] and/or evanescent waves [13–16] at short distances, are suggested to solve low-frequency problems, as well as multiscale problems involving large objects with dense discretizations.

In this work, we approach low-frequency breakdowns from a different direction and prevent them by using multiple-precision arithmetic (MPA), which has recently become popular in the scientific computation area [17, 18]. Considering breakdowns from a numerical point of view, the standard diagonalization of the Green's function fails to provide accurate subwavelength interactions due to insufficient numbers of digits used in computations. Even when using the double-precision arithmetic, plane waves can be insufficient to represent radiation and receiving patterns of small sources. In addition, translations at short distances may involve addition and subtraction of large numbers due to spherical Hankel functions. Increasing the number of digits by means of MPA, it becomes possible to improve all these computations and perform such critical interactions with a desired level of accuracy using the conventional diagonalization. MPA may easily be used in the existing implementations of MLFMA and convert them to broadband implementations via relatively simple modifications.

2. LOW-FREQUENCY BREAKDOWNS IN THE DIAGONALIZATION OF THE GREEN'S FUNCTION

Consider the truncated form of the Gegenbauer's addition theorem, i.e.,

$$g\left(\mathbf{r},\mathbf{r}'\right)=\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|}=\frac{\exp(ik|\mathbf{w}+\mathbf{v}|)}{4\pi|\mathbf{w}+\mathbf{v}|}=\frac{ik}{4\pi}\sum_{t=0}^{\tau}(-1)^t(2t+1)j_t(kv)h_t^{(1)}(kw)P_t(\hat{\mathbf{v}}\cdot\hat{\mathbf{w}}), \quad (1)$$

where k is the wavenumber, $\mathbf{r}-\mathbf{r}'=\mathbf{w}+\mathbf{v}$, $\mathbf{w}=\hat{\mathbf{w}}w$, $\mathbf{v}=\hat{\mathbf{v}}v$, and $w>v$. In the above, $h_t^{(1)}$ is the spherical Hankel function of the first kind, j_t is the spherical Bessel function of the first kind, and P_t represents Legendre polynomials. The truncation number τ is usually determined by heuristic approaches, such as excess bandwidth formulas [19]. MLFMA and similar fast algorithms are based on the diagonalization of the factorization in (1). For example, expanding spherical waves in terms of plane waves as

$$j_t(kv)P_t\left(\hat{\mathbf{v}}\cdot\hat{\mathbf{w}}\right)=\frac{1}{4\pi i^t}\int d^2\hat{\mathbf{k}}\exp(ik\hat{\mathbf{k}}\cdot\mathbf{v})P_t(\hat{\mathbf{k}}\cdot\hat{\mathbf{w}}), \quad (2)$$

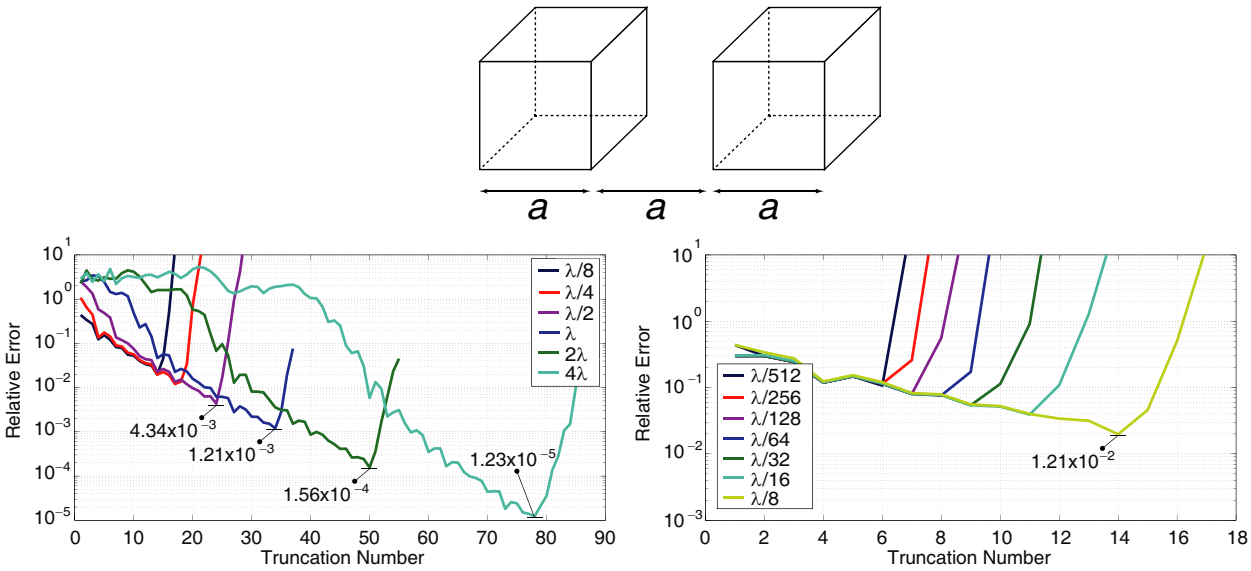

Figure 1: Maximum relative error in the diagonalized Green's function considering the worst-case scenario according to a one-box-buffer scheme for different box sizes. The standard double-precision arithmetic is used.

one can obtain

$$g\left(\mathbf{r},\mathbf{r}'\right)=\frac{ik}{(4\pi)^2}\sum_{t=0}^{\tau}i^t(2t+1)h_t^{(1)}(kw)\int d^2\hat{\mathbf{k}}\exp(ik\hat{\mathbf{k}}\cdot\mathbf{v})P_t(\hat{\mathbf{k}}\cdot\hat{\mathbf{w}}) \tag{3}$$

or

$$g\left(\mathbf{r},\mathbf{r}'\right)=\frac{ik}{(4\pi)^2}\int d^2\hat{\mathbf{k}}\exp(ik\hat{\mathbf{k}}\cdot\mathbf{v})\alpha_\tau(k,\hat{\mathbf{k}},\mathbf{w}), \tag{4}$$

where

$$\alpha_\tau(k,\hat{\mathbf{k}},\mathbf{w})=\sum_{t=0}^{\tau}i^t(2t+1)h_t^{(1)}(kw)P_t(\hat{\mathbf{k}}\cdot\hat{\mathbf{w}}) \tag{5}$$

represents the translation operator. We emphasize that (4) is typically used in MLFMA, while even the expression in (3) suffers from low-frequency breakdowns when $kw\ll 1$.

Figure 1 depicts a set of experiments, where we compute the relative error using the expression in (4) with respect to the direct evaluation of the Green's function. As also depicted in the figure, we consider cubic clustering (that is a standard in the conventional implementations of MLFMA [5]) and the worst-case scenario according to a one-box-buffer scheme. The box size (as well as the distance between boxes) is changed from 4λ to $\lambda/8$ and then from $\lambda/8$ to $\lambda/512$, whereas the truncation number (τ) is increased for each box size until a clear breakdown is observed. In these experiments, angular integrations are carried out by using $2(\tau+1)$ regular samples in the ϕ direction and $\tau+1$ Gauss-Legendre points in the θ direction [6]. For each case (box size and truncation number), we select the maximum error encountered in $15\times 15=225$ different scenarios considering different source and observation locations (including box centers, face centers, and corners). Given a box size, the error increases dramatically after an obvious breakdown, which occurs earlier for smaller boxes. It is remarkable that even 1% error cannot be achieved when the box size is smaller than $\lambda/8$, verifying that such box sizes are not suitable in MLFMA using the standard double-precision arithmetic.

There are many studies in the literature for solving low-frequency breakdowns in MLFMA. Two popular methods are using multipoles directly [8–12] and changing integration branches to complex angular values such that evanescent waves are included in subwavelength interactions [13–16]. Unfortunately, both types of methods require reimplementations of MLFMA in more complicated forms. In this study, we attack the low-frequency breakdown problem at a numerical level that leads to a straightforward solution to this important limitation. This new approach may also enable a direct implementation of a broadband MLFMA.

3. USING MPA TO PREVENT LOW-FREQUENCY BREAKDOWNS

MPA is well known in various areas [17], but is recently introduced in the computational electromagnetics community [18]. Using MPA, it is possible to use different precisions for representing different numbers. This is particularly useful when the double-precision arithmetic is not sufficient for accurate results. Low-frequency breakdowns in MLFMA can be interpreted as numerical problems due to disastrous effects of rounding errors. The spherical Hankel functions in (5) are very large when $kw \ll 1$ leading to difficult computations as new harmonics are added to achieve a convergence. In addition, radiation and receiving patterns of subwavelength boxes may not be expanded accurately via plane waves using the double-precision arithmetic. With more digits, how-

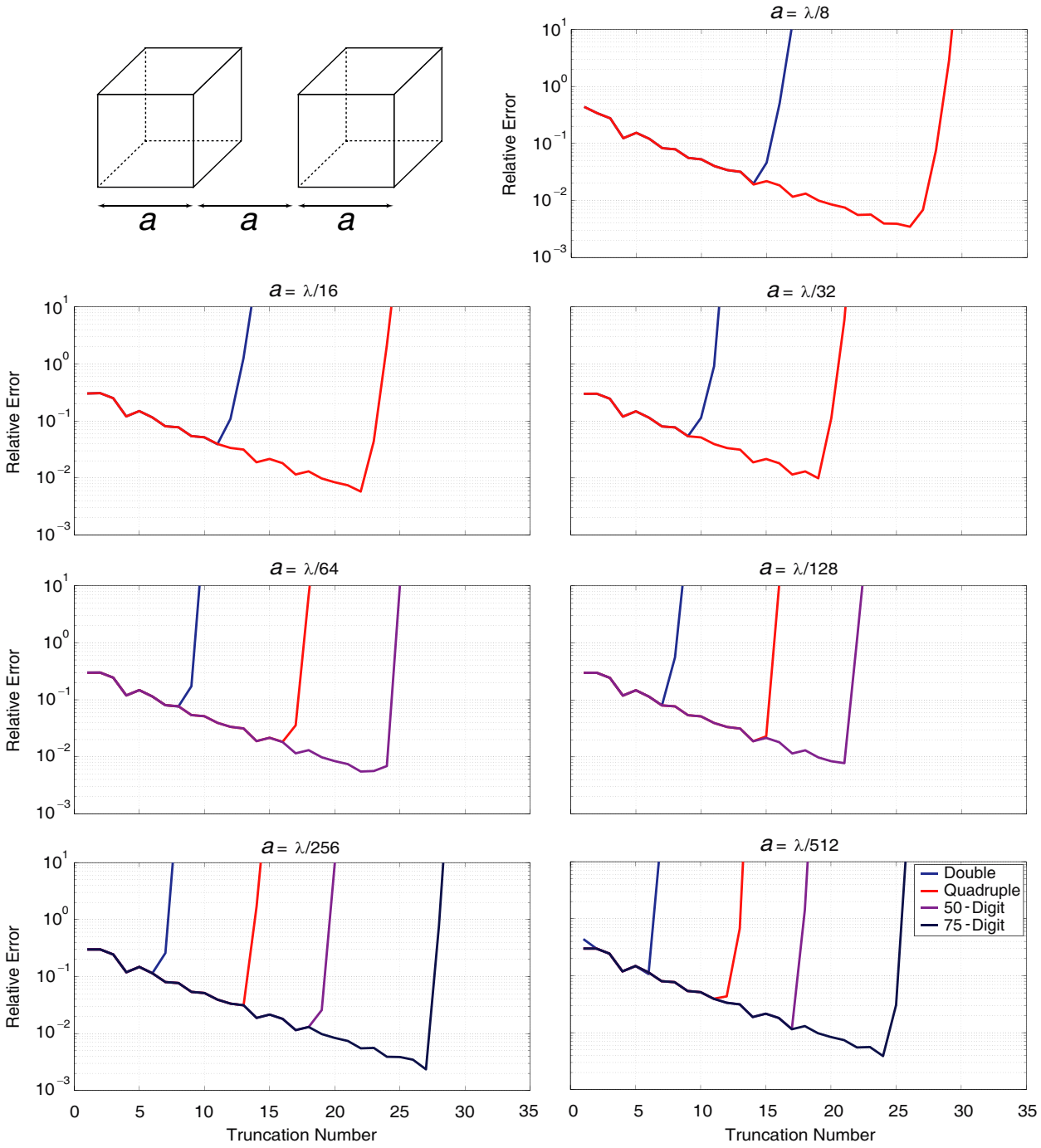

Figure 2: Maximum relative error in the diagonalized Green's function considering the worst-case scenario according to a one-box-buffer scheme. The box size is in the $\lambda/512 - \lambda/8$ range, while various precision arithmetics are used.

ever, it becomes possible to accurately represent patterns and add sufficient harmonics to achieve any desired level of accuracy.

As an example, Fig. 2 presents the results obtained when the box size is in the $\lambda/512 - \lambda/8$ range, while considering the worst case scenario according to a one-box-buffer scheme. We again select the maximum relative error encountered in $15 \times 15 = 225$ different cases as the truncation number increases from 1 to 35. It can be observed that using higher precision arithmetics delays the breakdown of the diagonalization. Specifically, the number of harmonics that can be used increases proportionally to the number of digits used in the computations, whereas the convergence rate is unaffected. By delaying the breakdown, we are able to use more harmonics to reduce the error and to improve the accuracy of the diagonalization.

Based on our experiments on the diagonalization of the Green's function using MPA, we are able to determine the number of harmonics as well as the precision required for a given box size and error criteria. As an example, Table 1 lists truncation numbers and precisions (number of digits) to achieve 1% maximum error for different box sizes from 4λ to $\lambda/512$. Maximum errors encountered in these measurements are also given in the fourth column. These values are again found by considering the worst case for boxes (see Figs. 1 and 2) and taking the maximum error out of 225 cases. We note that, in a typical solution using MLFMA, most of the interactions would require fewer harmonics and lower precisions, depending on locations of source and observation points in boxes. The following observations can be made in Table 1.

1. Double-precision arithmetic is sufficient only for boxes larger than $\lambda/4$ (shown with D in the third column), whereas smaller boxes require higher precisions to achieve 1% error.
2. For smaller boxes requiring higher precisions, halving the box size needs almost a constant increase in the number of digits to achieve the same diagonalization error. For 1% error, this corresponds to 5–6 digits.
3. For smaller boxes using higher precisions, the number of harmonics can be fixed, similar to low-frequency implementations using multipoles. For 1% diagonalization error, the truncation number can be fixed to 19.

Table 1: Truncation numbers and precisions required to obtain maximum 1% error in the diagonalization of the Green's function.

Box Size	Truncation Number	Precision (Digits)	Maximum Error
4λ	52	D	0.0095
2λ	30	D	0.0081
λ	23	D	0.0098
$\lambda/2$	20	D	0.0097
$\lambda/4$	19	19	0.0086
$\lambda/8$	19	24	0.0099
$\lambda/16$	19	29	0.0098
$\lambda/32$	19	34	0.0098
$\lambda/64$	19	40	0.0097
$\lambda/128$	19	46	0.0097
$\lambda/256$	19	52	0.0097
$\lambda/512$	19	57	0.0097

Numerical results, some of which are listed in Table 1, show that using MPA in the diagonalization of the Green's function provides a straightforward solution to low-frequency breakdowns. Hence, using MPA may extend the applicability of the conventional diagonalization, as well as MLFMA implementations, to multiscale problems. Using higher numbers of digits increases the cost, i.e., processing time and memory; but, the resulting solvers can still be efficient compared to other broadband implementations in the literature.

4. CONCLUSION

We use MPA to prevent low-frequency breakdowns in the diagonalization of the Green's function. This way, subwavelength interactions can be calculated accurately using the standard diagonal-

ization without resorting to alternative factorization and diagonalization methods. A systematic selection of precisions and their usage may be used to convert conventional MLFMA implementations to broadband solvers for solving multiscale problems.

ACKNOWLEDGMENT

This work was supported by the Scientific and Technical Research Council of Turkey (TUBITAK) under the Research Grant 113E276 and by a BAGEP Grant from Bilim Akademisi (The Science Academy, Turkey).

REFERENCES

1. Song, J., C.-C. Lu, and W. C. Chew, "Multilevel fast multipole algorithm for electromagnetic scattering by large complex objects," *IEEE Trans. Antennas Propag.*, Vol. 45, No. 10, 1488–1493, Oct. 1997.
2. Taboada, J. M., M. G. Araujo, J. M. Bertolo, L. Landesa, F. Obelleiro, and J. L. Rodriguez, "MLFMA-FFT parallel algorithm for the solution of large-scale problems in electromagnetics," *Progress In Electromagnetics Research*, Vol. 105, 15–30, 2010.
3. Ergül, Ö., "Solutions of large-scale electromagnetics problems involving dielectric objects with the parallel multilevel fast multipole algorithm," *J. Opt. Soc. Am. A.*, Vol. 28, No. 11, 2261–2268, Nov. 2011.
4. Ergül, Ö. and L. Gürel, "Fast and accurate analysis of large-scale composite structures with the parallel multilevel fast multipole algorithm," *J. Opt. Soc. Am. A.*, Vol. 30, No. 3, 509–517, Mar. 2013.
5. Chew, W. C., J.-M. Jin, E. Michielssen, and J. Song, *Fast and Efficient Algorithms in Computational Electromagnetics*, Artech House, Boston, MA, 2001.
6. Coifman, R., V. Rokhlin, and S. Wandzura, "The fast multipole method for the wave equation: A pedestrian prescription," *IEEE Antennas Propag. Mag.*, Vol. 35, No. 3, 7–12, Jun. 1993.
7. Koc, S., J. M. Song, and W. C. Chew, "Error analysis for the numerical evaluation of the diagonal forms of the scalar spherical addition theorem," *SIAM J. Numer. Anal.*, Vol. 36, No. 3, 906–921, 1999.
8. Zhao, J.-S. and W. C. Chew, "Three dimensional multilevel fast multipole algorithm from static to electrodynamic," *Microw. Opt. Technol. Lett.*, Vol. 26, No. 1, 43–48, Jul. 2000.
9. Zhao, J.-S. and W. C. Chew, "Applying LF-MLFMA to solve complex PEC structures," *Microw. Opt. Technol. Lett.*, Vol. 28, No. 3, 155–160, Feb. 2001.
10. Chu, Y.-H. and W. C. Chew, "A multilevel fast multipole algorithm for electrically small composite structures," *Microw. Opt. Technol. Lett.*, Vol. 43, No. 3, 202–207, Nov. 2004.
11. Jiang, L. J. and W. C. Chew, "A mixed-form fast multipole algorithm," *IEEE Trans. Antennas Propag.*, Vol. 53, No. 12, 4145–4156, Dec. 2005.
12. Ergül, Ö. and L. Gürel, "Efficient solutions of metamaterial problems using a low-frequency multilevel fast multipole algorithm," *Progress In Electromagnetics Research*, Vol. 108, 81–99, 2010.
13. Greengard, L., J. Huang, V. Rokhlin, and S. Wadzura, "Accelerating fast multipole methods for the Helmholtz equation at low frequencies," *IEEE Comput. Sci. Eng.*, Vol. 5, 32–38, Jul.–Sep. 1998.
14. Jiang, L. J. and W. C. Chew, "Low-frequency fast inhomogeneous plane-wave algorithm (LF-FIPWA)," *Microw. Opt. Technol. Lett.*, Vol. 40, No. 2, 117–122, Jan. 2004.
15. Bogaert, I., J. Peeters, and F. Olyslager, "A nondirective plane wave MLFMA stable at low frequencies," *IEEE Trans. Antennas Propag.*, Vol. 56, No. 12, 3752–3767, Dec. 2008.
16. Bogaert, I. and F. Olyslager, "A low frequency stable plane wave addition theorem," *J. Comput. Phys.*, Vol. 228, No. 4, 1000–1016, Mar. 2009.
17. Smith, D. M., "Using multiple-precision arithmetic," *Computing in Science and Engineering*, Vol. 5, No. 4, 88–93, Jul.–Aug. 2003.
18. Stefanski, T. P., "Electromagnetic problems requiring high-precision computations," *Antennas Propag. Mag.*, Vol. 55, No. 2, 344–353, Apr. 2013.
19. Ohnuki, S. and W. C. Chew, "Truncation error analysis of multipole expansions," *SIAM J. Sci. Comput.*, Vol. 25, No. 4, 1293–1306, 2003.