Error Analysis for the Truncation of Multipole Expansion of Vector Green's Functions

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***Abstract*—One of the most important mathematical formulas in fast multipole algorithms (FMA) is the addition theorem. In the numerical implementation of the addition theorem, the infinite series should be truncated. In this paper, the number of terms needed for the scalar Green's function is derived, and the error analysis for the truncation error in the multipole expansion of the vector Green's functions is given. We have found that the error term in vector Green's functions is proportional to $1/R$. If the scalar Green's function is truncated at the L-th term and the relative error is ϵ, then the relative error in the dyadic Green's function is $\epsilon/4$, if it is truncated at the $(L+2)$-th term. For the vector Green's function related to MFIE, the relative error is $\epsilon/2$ if it is truncated at the $(L+1)$-th term.**

***Index Terms*—Error analysis, fast multipole algorithms (FMA), vector Green's functions.**

I. INTRODUCTION

THE recent advent of fast algorithms in computational electromagnetics has permitted the solution of integral equations with an unprecedented number of unknowns. This is the consequence of the development of the fast multipole algorithms (FMA) [1] and the dynamic multilevel fast multipole algorithms (MLFMA) [2]. Such algorithms allow a matrix-vector multiplication to be performed in $O(N \log N)$ operations or less for many scattering problems. Moreover, the memory requirements of these methods are $O(N \log N)$, or almost matrix free. Using the fast matrix-vector multiplications in an iterative solver, problems for integral equations involving up to ten million unknowns have been solved recently [3]–[6].

One of the most important mathematical formulas in the FMA is the addition theorem. In the numerical implementation of the addition theorem, the infinite series should be truncated. The error analysis for the truncation error in the scalar Green's functions has been done by many researchers [1], [3] and [7]–[10]. In this paper, the number of terms needed for the scalar Green's function is derived, and the error analysis for the truncation error in the multipole expansion of the vector Green's functions is given.

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II. TRUNCATION ERROR IN SCALAR GREEN'S FUNCTION

The addition theorem for the scalar Green's function has the form [1]

$$g(R) = \frac{e^{ikR}}{kR} = \frac{e^{ik|\mathbf{D}+\mathbf{d}|}}{k|\mathbf{D}+\mathbf{d}|} \approx i\sum_{l=0}^{L}(-1)^l(2l+1)j_l(kd)h_l^{(1)}(kD)P_l(\hat{d}\cdot\hat{D}) \quad (1)$$

where $R = |\mathbf{r}-\mathbf{r}'| = |\mathbf{D}+\mathbf{d}|, \mathbf{r}$ and $\mathbf{r}'$ are for field and source points, $\mathbf{D}$ is a vector between two group centers, $\mathbf{d}$ is the summation of two local vectors [7], and $d < D, j_l(x)$ is a spherical Bessel function of the first kind, $h_l^{(1)}(x)$ is a spherical Hankel function of the first kind, and $P_l(x)$ is a Legendre polynomial.

The infinite series of (1) is truncated at the Lth term. The leading error term is $(2L+3)j_{L+1}(kd)/(kD)$ (for $L > kd$). Some researchers [1], [3] and [7]–[10] have given the semi-empirical formula

$$L \approx kd + \alpha \ln(\pi + kd) \quad (2)$$

where α is dependent on the accuracy; for example, $\alpha = 1$ gives the accuracy of 0.1 and $\alpha = 5$ results in 10^{-6} accuracy. Recently, Rokhlin derived a new formula for 2-D [11]

$$L \approx kd + \beta(kd)^{1/3} \quad (3)$$

where β is also dependent on the accuracy. The same formula was used in calculating the Mie series [12] and the optimal sampling of scattered fields [13]. For a given accuracy, we calculate the true L needed in (1), and then compare the true L with the values given by (2) and (3). In Fig. 1, we plot the differences between the approximated L and true L for an accuracy 10^{-6}. It is found that $kd + 5\ln(\pi + kd)$ is a good approximation for kd up to 40. But $kd + 6(kd)^{1/3}$ is always a good approximation.

Let us derive β as a function of the accuracy requirement. The relative error in the truncated scalar Green's function of (1) can be written as

$$\epsilon = kR\left|\sum_{l=L+1}^{\infty}(-1)^l(2l+1)j_l(kd)h_l^{(1)}(kD)P_l(\hat{d}\cdot\hat{D})\right|. \quad (4)$$

The error in each term of (4) is maximum when $\mathbf{D}$ and $\mathbf{d}$ are collinear [10]. Applying the large argument approximation of the spherical Hankel function, we have

$$\epsilon \approx \frac{R}{D}\left|\sum_{l=L+1}^{\infty} i^l(2l+1)j_l(kd)\right| \approx (2L+3)j_{L+1}(kd) \quad (5)$$

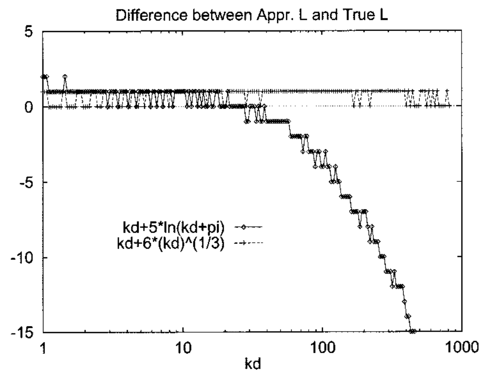

Fig. 1. Differences between the L calculated using $kd + 5\ln(\pi + kd)$, or $kd + 6(kd)^{1/3}$, and true L for an accuracy 10^{-6}.

where only the leading error term is kept. With large order and argument, $j_{L+1}(kd)$ can be approximated as [14]

$$j_{L+1}(x) \approx \frac{1}{2\sqrt{f(L,x)x}} e^{f(L,x)-(L+3/2)\ln\{[L+3/2+f(L,x)]/x\}} \quad (6)$$

where $x = kd$, and $f(L,x) = [(L+3/2)^2 - x^2]^{1/2}$. Let us change the variable using

$$L + \frac{3}{2} = x(1+\delta). \quad (7)$$

Since the spherical Bessel function decreases very fast when the order is larger than the argument, δ is very small compared to x. So we have the approximations

$$\epsilon \approx (2\delta)^{-1/4} e^{-x(2\delta)^{3/2}/3}. \quad (8)$$

The second factor in (8) is much smaller than the first factor and hence dominates when the log of (8) is taken. Therefore, we have

$$\delta \approx \frac{1}{2}\left[\frac{3\ln(1/\epsilon)}{x}\right]^{2/3} = 1.8\left[\frac{\log(1/\epsilon)}{x}\right]^{2/3}. \quad (9)$$

Finally, we have a more refined formula

$$L \approx kd + 1.8 d_0^{2/3}(kd)^{1/3} \quad (10)$$

where $d_0 = \log(1/\epsilon)$, which is very close to the number of digits of accuracy, Int$[\log(1/\epsilon) + 1.0 - \log(2)]$. Equation (10) is a very good approximation. For kd varying from 1 to 500, ϵ varies from 10^{-1} to 10^{-10}, the difference between the approximated L and true L is between -1 and 2.

III. Truncation Error in the Vector Green's Function

Applying the addition theorem (1) to the dyadic Green's function, and expanding the spherical wave in plane waves yield [1], [7]

$$\bar{\mathbf{G}}(\mathbf{r},\mathbf{r}') \approx \int d^2\hat{k}(\bar{\mathbf{I}} - \hat{k}\hat{k}) e^{i\mathbf{k}\cdot\mathbf{d}} \alpha_L(\hat{D}\cdot\hat{k}) \quad (11)$$

where $\alpha_L(\hat{D}\cdot\hat{k}) = (i/4\pi)\sum_{l=0}^{L} i^l(2l+1)h_l^{(1)}(kD)P_l(\hat{D}\cdot\hat{k})$. Expanding $\bar{\mathbf{I}} - \hat{k}\hat{k}$ in Cartesian coordinates, we have

$$\begin{aligned}\bar{\mathbf{I}} - \hat{k}\hat{k} = &(1 - \sin^2\theta\cos^2\phi)(\hat{x}\hat{x} + \hat{y}\hat{y}) + \sin^2\theta\hat{z}\hat{z}\\ &- \sin^2\theta\sin\phi\cos\phi(\hat{x}\hat{y} + \hat{y}\hat{x})\\ &- \sin\theta\cos\theta\cos\phi(\hat{x}\hat{z} + \hat{z}\hat{x})\\ &- \sin\theta\cos\theta\sin\phi(\hat{y}\hat{z} + \hat{z}\hat{y}).\end{aligned} \quad (12)$$

The error in (1) and (11) is maximum when $\mathbf{D}$ and $\mathbf{d}$ are collinear [10]. To simplify our analysis, we assume that both $\mathbf{D}$ and $\mathbf{d}$ are along the z-axis and replace $\cos\theta$ with x. So the components of the dyadic Green's function in Cartesian coordinates are given by

$$\begin{aligned}G_{zz} &= 2\pi\int_{-1}^{1} dx(1-x^2)\alpha_L(x)e^{ixkd}\\ G_{yy} &= G_{xx} = g(R) - G_{zz}/2\\ G_{xy} &= G_{yx} = G_{xz} = G_{zx} = G_{yz} = G_{zy} = 0.\end{aligned} \quad (13)$$

There are three nonzero diagonal components, too. G_{zz} is the radial component and should not have the $1/R$ term. G_{xx} and G_{yy} are the transverse components. To check the error term in G_{zz} of (13), we use the expansion of a plane wave to spherical waves $[e^{ixkd} = \sum_{n=0}^{\infty} i^n(2n+1)j_n(kd)P_n(x)]$, the translation $\alpha_L(x) = i/4\pi\sum_{l=0}^{L} i^l(2l+1)h_l^{(1)}(kD)P_l(x)$, the recurrence relations for Legendre polynomials $[xP_l(x)$ and $x^2P_l(x)]$, and the asymptotic form of $h_l^{(1)}(kD)$ for large kD [14]. Then we have

$$\begin{aligned}G_{zz} \approx &\frac{e^{ikD}}{2kD}\sum_{n=0}^{\infty} i^n(2n+1)j_n(kd)\sum_{l=0}^{L}\int_{-1}^{1} dxP_n(x)\\ &\times\left\{\frac{l(l-1)}{2l-1}[P_l(x) - P_{l-2}(x)] + \frac{(l+1)(l+2)}{2l+3}\right.\\ &\left.\times[P_l(x) - P_{l+2}(x)]\right\}.\end{aligned} \quad (14)$$

Using the orthogonality of Legendre polynomials, we find that $G_{zz} = 0$ (no $1/D \approx 1/R$ term) when $L \to \infty$. But when FMA truncates the series at the Lth term, the leading order error term in G_{zz} is $(L(L+1))/(2L+1)j_{L-1}(kd)/(kD)$. Similarly, the leading order error term in G_{xx} and G_{yy} is found to be $[(2L+3)j_{L+1}(kd) - (L(L+1))/(2(2L+1))j_{L-1}(kd)]/(kD)$. For small kd, L is much larger than kd, and the second term is dominant. So, if the scalar Green's function is truncated at the Lth term and the relative error is ϵ, then the relative error of the transverse components of the dyadic Green's function is approximately $\epsilon/8$ if it is truncated at the $(L+2)$-th term. For the radial component, the relative error normalized by the transverse component is $\epsilon/4$ if it is truncated at the $(L+2)$-th term. The relative error normalized by itself is $kR\epsilon/8$. Therefore, the relative error of the dyadic Green's function is $\epsilon/4$.

The vector Green's function for the magnetic field integral equation (MFIE) is just the gradient of the scalar Green's function

$$\nabla g(R) = k[i - 1/(kR)]g(R)\hat{R}. \quad (15)$$

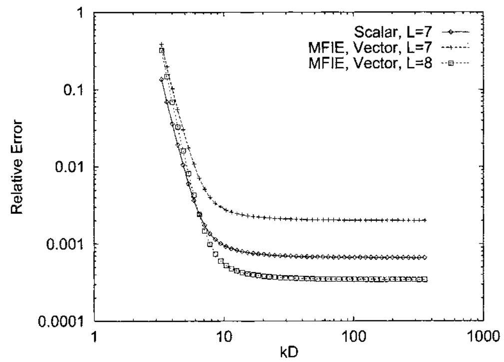

Fig. 2. Relative truncation errors of the scalar Green's function and vector Green's function for the MFIE $[\nabla g(R)]$ for $\mathbf{D} = D\hat{z}$ and $\mathbf{d} = 0.4\lambda\hat{z}$.

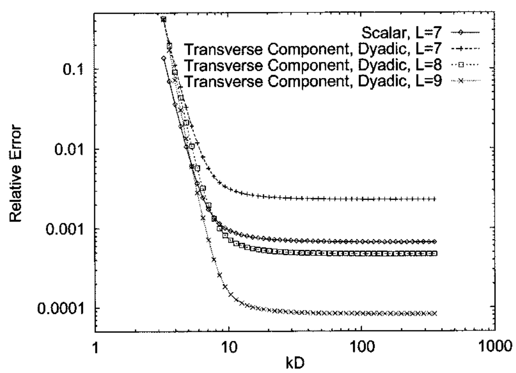

Fig. 3. Relative truncation errors of the scalar Green's function, and the transverse component of the dyadic Green's function for $\mathbf{D} = D\hat{z}$ and $\mathbf{d} = 0.4\lambda\hat{z}$.

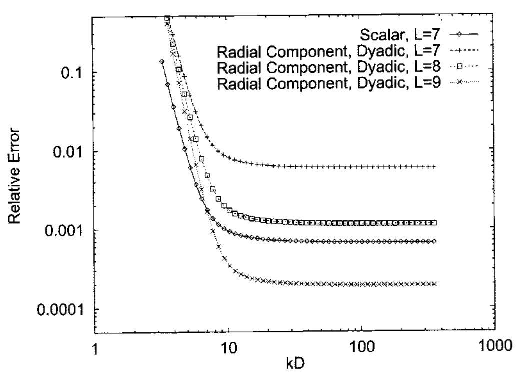

Fig. 4. Relative truncation errors of the scalar Green's function and the radial component (normalized by the transverse component) of the dyadic Green's function for $\mathbf{D} = D\hat{z}$ and $\mathbf{d} = 0.4\lambda\hat{z}$.

Its FMA factorization can be written as [15]

$$\nabla g(R) \approx \int d^2\hat{k}\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{d}}\alpha_L(\hat{D}\cdot\hat{k}). \tag{16}$$

Using the above analysis, we find that the leading error term in $\nabla g(R)$ is $(L+1)j_L(kd)/(kD)$. So, the relative accuracy is $\epsilon/2$ if it is truncated at the $(L+1)$-th term.

In Fig. 2, we plot the relative truncation errors of the scalar Green's function and the vector Green's function for the MFIE $[\nabla g(R)]$. It is found that if the vector Green's function retains one more term than the scalar Green's function, the truncation error of the vector Green's function is one half the error of the scalar Green's function. Corresponding to the above analysis, the relative errors of the transverse and radial components of the dyadic Green's function are plotted in Figs. 3 and 4. The error for the radial component is normalized by the transverse component. If the dyadic Green's function retains two more terms than the scalar Green's function, the radial component has $1/4$ of the error of the scalar Green's function and the transverse component has $1/8$ of the error, as indicated by the above analysis.

IV. Conclusion

If the number of digits of accuracy in the truncated Green's function is d_0, the number of terms is given by $L = kd + 1.8d_0^{2/3}(kd)^{1/3}$. We also analyze the truncation error in the FMA expansion of the vector Green's function. The error term in the vector Green's function is proportional to $1/R$. If the scalar Green's function is truncated at the Lth term and the relative error is ϵ, then the relative error in the dyadic Green's function is $\epsilon/4$ if it is truncated at the $(L+2)$-th term. For the vector Green's function related to MFIE, the relative error is $\epsilon/2$ if it is truncated at the $(L+1)$-th term.

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