On the Lagrange Interpolation in Multilevel Fast Multipole Algorithm

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Introduction

We consider the Lagrange interpolation employed in the multilevel fast multipole algorithm (MLFMA) [1] as part of our efforts to obtain faster and more efficient solutions for large problems of computational electromagnetics. For the translation operator, we present the choice of the parameters for optimal interpolation. For the aggregation and dissaggregation processes, we discuss the interpolation matrices and introduce an efficient way of improving the accuracy by employing the poles.

Lagrange Interpolation

For a scalar field $f(\theta, \phi)$ as a function of the spherical coordinates, 2-D Lagrange interpolation can be written as

$$\tilde{f}(\theta, \phi) = \sum_{i=s+1-p}^{s+p} w_i(\phi) \sum_{j=t+1-p}^{t+p} v_j(\theta) f(\theta_j, \phi_i), \tag{1}$$

where θ_j and ϕ_i are the coordinates of the sampling points on the coarse grid and $\tilde{f}(\theta, \phi)$ represents the value of the field at (θ, ϕ), perturbed by the interpolation error. Interpolation weights are derived as

$$w_i(\phi) = \prod_{\substack{k=s+1-p \\ k \neq i}}^{s+p} \frac{\phi - \phi_k}{\phi_i - \phi_k}, \qquad v_j(\theta) = \prod_{\substack{l=t+1-p \\ l \neq j}}^{t+p} \frac{\theta - \theta_l}{\theta_j - \theta_l} \tag{2}$$

for the ϕ and θ directions, respectively. In (1), the interpolation at (θ, ϕ) is performed by employing $2p \times 2p$ points located at (θ_j, ϕ_i).

Optimal Lagrange Interpolation of the Translation Operator

In the MLFMA, as in the fast multipole method (FMM), the interactions between the clusters are performed by the translation operators that are defined as

$$T(k, D, \varphi) = \frac{ik}{4\pi} \sum_{l=0}^{L} (i)^l (2l + 1) h_l^{(1)}(kD) P_l(\varphi), \tag{3}$$

where $h_l^{(1)}$ is the spherical Hankel function of the first kind, P_l is the Legendre polynomial, and L is the truncation number. For a clustering scheme employing a regular grid, where the box size is fixed for each level, symmetry of the translations leads to a significant reduction in the number of the translation operators required in a solution

TABLE I
SPEED-UP OBTAINED USING THE OPTIMAL (p, s) PAIR FOR $a \geq 4\lambda$

d_0	(p, s)	$a = 4\lambda$	$a = 8\lambda$	$a = 16\lambda$	$a = 32\lambda$	$a = 64\lambda$
2	(2,3.5)	14.0	27.5	54.3	108.3	216.0
3	(2,6.5)	10.8	20.2	40.0	77.0	151.9
4	(3,6.0)	7.9	15.0	28.9	56.9	113.7
5	(3,8.5)	7.1	13.0	24.7	48.4	96.6

by the MLFMA [2]. However, a direct calculation of the operators requires $O(N^{3/2})$ processing time, which becomes substantial as the problem size grows. As a remedy, a two-stage method is suggested [3], where the translation operator in (3) is sampled at $O(N)$ points as a function of φ, and then it is evaluated at the required points by a Lagrange interpolation. Since the translation operator is a band-limited function of φ and the Lagrange interpolation is local, i.e., interpolation at a point requires $2p \times 2p$ samples in the neighborhood, the method reduces the complexity to $O(N)$ with small interpolation error. In [3], the interpolation parameters, namely the number of interpolation points p and the over-sampling factor s, are fixed to 3 and 5.0, respectively. In this paper, we further improve the interpolation by optimizing these parameters.

In Table I, we present the optimal selection of the interpolation parameters and the resulting speed-up compared to the direct method. As depicted in Figs. 1(a) and (b), we employ the optimized pairs of (p, s) to obtain the desired level of accuracy with the minimum processing time. This is demonstrated for the case of two interacting clusters separated by $\boldsymbol{D} = \hat{\boldsymbol{x}}2a$ and a changes from 4λ to 64λ. However, the optimal p and s are obtained by considering all the possible cases in the MLFMA. The number of accurate digits, d_0, for the FMM interactions changes from 2 to 5, and we desire to obtain an interpolation error lower than the FMM error. The errors and the speed-up provided by the fixed $p = 3, s = 5.0$ are also plotted on the same figures. Comparisons show that

- the fixed case satisfies the desired level of accuracy for $d_0 = 2, 3$, however, the optimized (p, s) gives better speed-up for these values of d_0,
- the fixed case seems to give better speed-up for $d_0 = 4, 5$, but in fact the accuracy is not in the desired levels, i.e., the interpolation error exceeds the FMM error.

Therefore, it is essential to optimize p and s in the Lagrange interpolation of the translation operators for both controllable accuracy and improved efficiency.
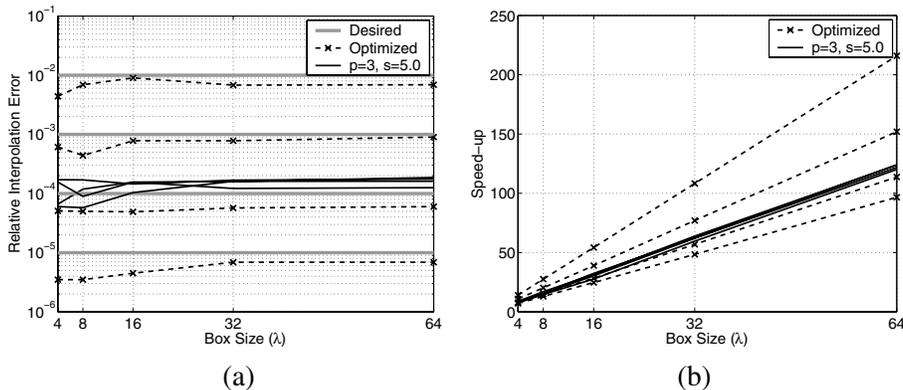

Fig. 1. (a) Interpolation error and (b) corresponding speed-up for different box sizes from 4λ to 64λ and for $d_0 = 2, 3, 4, 5$. ($\boldsymbol{D} = \hat{\boldsymbol{x}}2a$)

TABLE II

PEAK MEMORY AND SOLUTION TIME OF THE PARALLEL MLFMA EMPLOYING
MEMORY-EFFICIENT (ME) AND TIME-EFFICIENT (TE) INTERPOLATION SCHEMES

Problem	Unknowns	Iterations	ME Interpolation	TE Interpolation
Sphere (Radius = 20λ)	1,462,854	29	694 MB, 18677 sec	736 MB, 10121 sec
Thin Box ($0.4\lambda \times 6\lambda \times 90\lambda$)	213,225	62	247 MB, 14116 sec	402 MB, 4412 sec

Lagrange Interpolation in the Aggregation and Disaggregation

In the aggregation (disaggregation) process of the MLFMA, interpolation (anterpolation) operations are performed between levels to match the sampling rates for the radiating (incoming) waves. Different sampling rates are required for different levels due to the nature of the Helmholtz equation, i.e., the number of multipoles required to satisfy a level of accuracy is related to the size of the region containing the sources. Therefore, larger clusters in the upper levels of the MLFMA require finer samplings compared to the small clusters in the lower levels. Due to the adjusted sampling rate based on the harmonic content, a fixed number of interpolation points $2p \times 2p$ is sufficient to obtain the same level of accuracy for all levels.

For the case of clustering using a regular grid, a single interpolation matrix is sufficient to perform all the interpolations from any level to the next level. Since the Lagrange interpolation is local, the interpolation matrices are sparse. Generally, a $K \times K$ matrix has $4Kp$ nonzero elements, where p is usually between 2 and 5, and $K = 2(L + 1)^2$, where L is the truncation number. As presented in Table II for the two large scattering problems solved on a 32-processor Pentium-4 parallel system, there are two schemes to perform the interpolations. In the memory-efficient scheme, the interpolation matrices are not formed explicitly, but the matrix elements are recalculated each time they are required. This scheme is useful for avoiding the storage of large interpolation matrices, especially if the number of levels is high. When the memory is not critical, it is possible to switch to time-efficient algorithm, where the interpolation matrices are calculated once and stored in the memory.

The Use of Poles in the Lagrange Interpolation

Finally, we present an efficient way to improve the accuracy of the Lagrange interpolation (anterpolation) during the aggregation (disaggregation) process of the MLFMA. Fig. 2(a) depicts a practical case related to an aggregation step from the lowest level of the MLFMA with the cluster size of 0.25λ to the next level with the cluster size of 0.5λ. We consider an interpolation to a point (star) on the fine grid with the location in spherical coordinates $(\theta, \phi) = (0.409, 0.483)$ given in radians. The number of interpolation points is 4×4 and they are represented by the shaded circles. We note that the samples are regularly spaced in the ϕ direction, but they are chosen as the Gauss-Legendre points in the θ direction. It can be observed that the topmost row of the 4×4 interpolation grid has a negative θ value, i.e., the points with $\theta = -0.253$ are employed in the interpolation. In other words, the next sample after $\theta = 0.253$ in the decreasing θ direction is on the other side of the $\theta = 0$ point, which is the north pole of the sphere. Consequently, there exists a wide gap in the θ direction, namely $2 \times 0.253 = 0.506$ radians. These wide gaps are responsible for

the larger interpolation errors at the points near the poles compared to the other points around the equator.

To reduce the interpolation error described above, we sample the fields at $\theta = 0$ and $\theta = \pi$, although these points do not contribute to the angular integration. We evaluate and store the vector field at the poles in the x and y directions. In this scheme, θ and ϕ components are extracted as

$$\begin{bmatrix} \hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{\phi}} \end{bmatrix} \cdot \boldsymbol{f}_{r/i}(0, \phi) = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \cdot \begin{bmatrix} \hat{\boldsymbol{x}} \cdot \boldsymbol{f}_{r/i} \\ \hat{\boldsymbol{y}} \cdot \boldsymbol{f}_{r/i} \end{bmatrix} \tag{4}$$

whenever required for the interpolation. This simple technique provides a significant improvement in the accuracy. In Fig. 2(b), the relative interpolation error for the θ component of the field, which is introduced during an aggregation process from the lowest level to the fourth level (from the bottom), is plotted with respect to the samples. The additional error around the pole locations (corresponding to the left and right sides of the figure) is eliminated by employing the poles. The extra cost of this technique in the MLFMA is negligible compared to the overall aggregation and disaggregation processes.
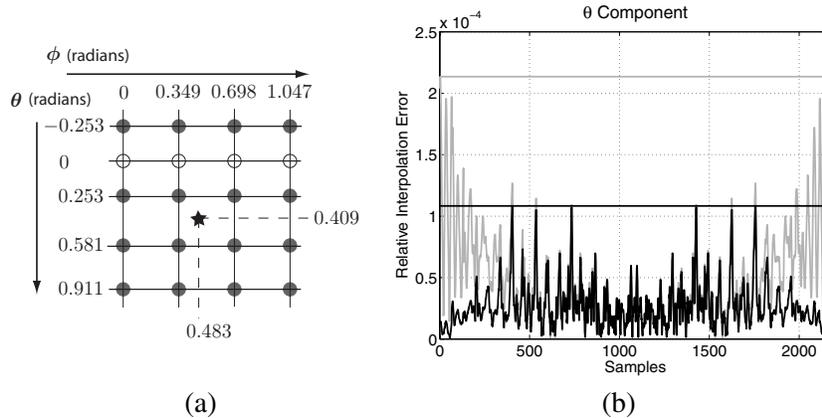

Fig. 2. Lagrange interpolation employing 4×4 points (shaded circles) located on the coarse grid to evaluate the function at a point (star) located on the fine grid. (b) Interpolation error obtained with the use of the poles (dark) and without the poles (light). Samples on a 33×66 grid are converted into one-dimensional data by a row-wise arrangement of the θ-ϕ space.

Conclusion

In conclusion, we investigate the use of the Lagrange interpolation in the MLFMA. The optimal interpolation of the translation operator is presented and an efficient technique is introduced for improved accuracy of the aggregation and disaggregation processes.

References

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