A Complexity-Reduced $\mathcal{H}$-Matrix Based Direct Integral Equation Solver with Prescribed Accuracy for Large-Scale Electrodynamic Analysis

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Introduction

The Integral equation (IE) based computational electromagnetic methods generally lead to a dense system of linear equations, the solution of which could be very expensive. Recently, fast solvers [1-3] such as FMM-based methods, fast low-rank compression methods, FFT-based methods, and $\mathcal{H}^2$-matrix based methods have been developed, which dramatically reduce the memory and CPU time of iterative IE solvers for electrodynamic problems. Fast direct solvers have also been developed. LU factorization of $O(N^2)$ time complexity and $O(N^{1.5})$ memory complexity was reported [4]. Compared to iterative solvers, direct solvers have advantages when the number of iterations or the number of right hand sides is large.

In this work, by further developing the $\mathcal{H}$−matrix [5] based mathematical framework, we achieved an efficient LU-factorization based direct IE solver of $k_{ave}^2 C_{sp}^2 O(N\log^2 N)$ time complexity and $k_{ave} C_{sp} O(N\log N)$ memory complexity, with the two parameters k_{ave} and C_{sp} minimized, with the prescribed accuracy satisfied, to solve large-scale electrodynamic problems. The k_{ave} is a weighted average rank we introduce to derive the complexity bounds for the $\mathcal{H}$-matrix-based computation of electrodynamic problems. It is introduced based on the fact that the rank required by an electrodynamic system for a given accuracy is a variable with respect to tree levels and admissible blocks, and hence existing constant-rank based complexity analysis does not apply. To minimize k_{ave} for a given accuracy, we develop an efficient method to determine a minimal rank for each admissible block. To minimize sparsity constant C_{sp} for a given accuracy, we develop an algorithm to optimize the $\mathcal{H}$-partition, in which we show that the existing admissibility condition based $\mathcal{H}$-partition is empirical instead of theoretical, and hence not optimal for a given accuracy and a given frequency. The proposed direct IE solver successfully factorizes dense matrices that involve more than 1 million unknowns associated with 96 wavelengths in fast CPU time (less than 20 hours in factorization and 85 seconds in solution on a single 8222SE AMD Opteron processor), modest memory consumption (less than 37.6 GB), and with the prescribed accuracy satisfied. It is kernel independent, and hence applicable to any IE-based formulation.

Background

Consider a dense system of linear equations $\mathbf{G}I = V$. An $\mathcal{H}$-based representation of $\mathbf{G}$ is associated with an admissibility condition. To define an admissibility condition, we denote the whole index set containing the basis functions used for discretization by $\mathcal{I} := \{1, 2, \ldots, N\}$. Consider two subsets t and s of $\mathcal{I}$, the admissibility condition is defined as [5, p.32-33]

$$(t,s) \text{ are admissible if } \min\{diam(Q_t), diam(Q_s)\} \le \eta dist(Q_t, Q_s), \tag{1}$$

where η is a positive parameter that can be used to control the admissibility condition. In an $\mathcal{H}$-matrix representation, an inadmissible block keeps its original full-matrix representation; while an admissible block has a factorized low-rank form. To be specific, an admissible block $\mathbf{G}^{t,s}$ formed by subsets t and s can be written as a factorized form $\mathbf{G}^{t,s}_{m,n} = \mathbf{A}_{m,k}\mathbf{B}^{\mathrm{T}}_{n,k}$, (2)

where $k \in \mathbb{N}$ is the rank of $\mathbf{G}^{t,s}$. If all the blocks $\mathbf{G}^{t,s}$ formed by the admissible (t,s) in $\mathbf{G}$ can be represented by a factorized form (2), $\mathbf{G}$ has an $\mathcal{H}$-matrix representation ([5], p. 18).

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Proposed Complexity Bounds for $\mathcal{H}$-Based Electrodynamic Analysis

For an electrodynamic problem, to satisfy a prescribed accuracy, the rank, in general, is not a constant with respect to admissible blocks and tree levels. Therefore, the complexity analysis of $\mathcal{H}$-based computations based on a constant rank given in [5] need to be re-derived for electrodynamic problems. We thus introduce weighted average rank k_{ave}, and define it as:

$$k_{ave} = \sum_{i=1}^{nk} k_i (m_i + n_i) / \sum_{i=1}^{nk} (m_i + n_i) \tag{3}$$

where nk is the total number of admissible blocks, k_{i} is the rank of the i-th admissible block, m_{i} and n_{i} are the number of rows and columns of the admissible block. The weighted average rank can be used to effectively bound the complexity of $\mathcal{H}$-based computations without overestimating the complexity. To explain, in an $\mathcal{H}$ matrix, each admissible block $\mathbf{G}^{m_i \times n_i}$ has a factorized form $\mathbf{A}^{m_i \times k_i}\mathbf{B}^{n_i \times k_i}$ with rank k_i. The storage is hence reduced from $m_i \times n_i$ units to $k_i(m_i + n_i)$ units. By summing up the storage of all the admissible blocks, we obtain

$$\text{Storage} = \sum_{i=1}^{nk} k_i (m_i + n_i) \overset{based\ on\ (3)}{=} k_{ave} \sum_{i=1}^{nk} (m_i + n_i) \overset{[6],\ p.\ 125,\ Lemma\ 7.4}{\leq} k_{ave} C_{sp} O(N \log N), \tag{4}$$

where C_{sp} is the maximal number of blocks that can be formed by a cluster in a block cluster tree. Similarly, we can use the average rank (3) to bound the time complexity of the $\mathcal{H}$-based computations. Take the matrix-matrix multiplication as an example, the cost for each admissible block involved in the multiplication is $C_{sp} k_i^2 (m_i + n_i)$ ([5], pp. 127-130). By summing up the cost of all the admissible blocks across all the tree levels, we obtain

$$\begin{aligned} &\text{Time Complexity} = C_{sp} \sum_{l=0}^{P} \sum_{i=1}^{nk} k_i^2 (m_i + n_i) \leq C_{sp} \sum_{l=0}^{P} k_{\max} \sum_{i=1}^{nk} k_i (m_i + n_i) \leq C_{sp} k_{\max} \sum_{l=0}^{P} (\text{Storage}) \\ &\leq C_{sp}^2 k_{\max} k_{ave} O(N \log^2 N) \overset{k_{\max} \propto O(k_{ave})}{=} C_{sp}^2 k_{ave}^2 O(N \log^2 N) \end{aligned}, \tag{5}$$

where $k_{\max}$ is the maximal rank among all the admissible blocks, which is an $O(k_{ave})$ quantity, and P is the tree depth that is proportional to $\log N$.

Proposed Methods for Reducing the Complexity of $\mathcal{H}$-Matrix Based Direct Solution

From (4) and (5), it can be seen clearly that to reduce the computational cost of an $\mathcal{H}$-based electrodynamic analysis, we have to reduce k_{ave} and C_{sp}. In the following two subsections, we present methods for reducing k_{ave}, and C_{sp} respectively.

A. Proposed method for minimizing average rank k_{ave} based on a prescribed accuracy

To minimize k_{ave}, for each admissible block, we determine a minimal rank based on a prescribed accuracy. Given an accuracy requirement, singular value decomposition (SVD) is the most accurate method to obtain the minimum rank that can meet the accuracy requirement for an admissible block. However, if we directly apply SVD to the original full matrix to obtain its $\mathcal{H}$-matrix representation, the computational cost is high. We then first use ACA+ ([5], pp. 71-74) which is a variant of ACA to efficiently compute an $\mathcal{H}$-matrix representation. The output of ACA+ algorithm has a form (2).We then apply reduced SVD ([5], p. 108) to the $\mathcal{H}$-matrix representation to determine the actual rank that is needed to satisfy the accuracy requirement ε. The resultant rank is minimal, and meanwhile it is obtained in linear complexity for each block. The effectiveness of the proposed scheme for rank minimization is shown in Fig. 1, which plots the rank distributions with the proposed scheme and with ACA+ only. It can be seen that by using the proposed method, the rank in most admissible blocks is reduced by half.

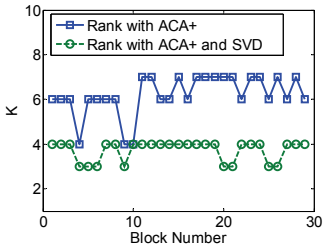

Fig. 1 Rank distribution in the lowest level with $\varepsilon = 10^{-4}$

Moreover, the same accuracy, measured by $\|\mathbf{G}-\tilde{\mathbf{G}}\|_F / \|\mathbf{G}\|_F$, is achieved. The accuracy is 1.02×10^{-5} and 1.08×10^{-5} without and with the rank minimization, respectively.

B. Proposed method for optimizing $\mathcal{H}$-matrix partition to reduce C_{sp}

The approach in the above section is performed based on an $\mathcal{H}$-matrix partition pre-determined by (1). If this partition is optimal for a given accuracy, i.e. resulting in a smallest C_{sp} for a given accuracy, then there is no need to investigate other partition schemes. However, in reality, the $\mathcal{H}$-matrix partition determined by (1) is not an optimal one. This can also be understood easily from the fact that the admissibility condition (1) is frequency independent. The admissibility condition given in (1) is empirical instead of theoretical. It is controlled by an empirical parameter η, instead of a prescribed accuracy. Therefore, we propose a new algorithm as shown in (6) to optimize the $\mathcal{H}$-matrix partition based on a prescribed accuracy ε_{opt}. The resultant $\mathcal{H}$-matrix partition significantly reduces the sparsity constant C_{sp}. In (6), the function **Rk Factor** is to factorize a full-matrix block to a rank-k matrix shown in (2) based on a prescribed accuracy. The function **Merge Rkblocks** is to merge multiple small admissible blocks to a single one based on the prescribed accuracy. To give an example, four admissible sub-blocks can be merged into one admissible block as follows.

Proposed Partition Optimization

Procedure $\mathcal{H}$-$\mathcal{P}_{\text{opt}}$ ($\mathcal{P}$) (Input $\mathcal{P}$ is the original $\mathcal{H}$-partition, output $\mathcal{P}$ is overwritten by an optimized $\mathcal{H}$-partition)

if $\mathcal{P}$ is a non-leaf off-diagonal matrix block

  for (i=0;i<4;i++)

    if $\mathcal{P}(i)$ is inadmissible block

      Rk_factor($\mathcal{P}(i)$, ε_{opt}) (6)

    if $\mathcal{P}(i)$ is a non-leaf block

      $\mathcal{H}$-$\mathcal{P}_{\text{opt}}$ ($\mathcal{P}(i)$, ε_{opt});

  if all blocks in $\mathcal{P}$ are admissible blocks

    Merge_Rkblocks($\mathcal{P}$, ε_{opt})

$$\begin{bmatrix}\mathbf{A}_1\mathbf{B}_1^{\mathrm{T}} & \mathbf{A}_2\mathbf{B}_2^{\mathrm{T}}\\ \mathbf{A}_3\mathbf{B}_3^{\mathrm{T}} & \mathbf{A}_4\mathbf{B}_4^{\mathrm{T}}\end{bmatrix}=\begin{bmatrix}\mathbf{A}_1\\0\end{bmatrix}\begin{bmatrix}\mathbf{B}_1\\0\end{bmatrix}^{\mathrm{T}}+\begin{bmatrix}\mathbf{A}_2\\0\end{bmatrix}\begin{bmatrix}0\\\mathbf{B}_2\end{bmatrix}^{\mathrm{T}}+\begin{bmatrix}0\\\mathbf{A}_3\end{bmatrix}\begin{bmatrix}\mathbf{B}_3\\0\end{bmatrix}^{\mathrm{T}}+\begin{bmatrix}0\\\mathbf{A}_4\end{bmatrix}\begin{bmatrix}0\\\mathbf{B}_4\end{bmatrix}^{\mathrm{T}}=\tilde{\mathbf{A}}_1\tilde{\mathbf{B}}_1^{\mathrm{T}}+\tilde{\mathbf{A}}_2\tilde{\mathbf{B}}_2^{\mathrm{T}}+\tilde{\mathbf{A}}_3\tilde{\mathbf{B}}_3^{\mathrm{T}}+\tilde{\mathbf{A}}_4\tilde{\mathbf{B}}_4^{\mathrm{T}}\overset{\varepsilon_{opt}}{=}\mathbf{A}\mathbf{B}^{\mathrm{T}}$$

where the addition in the final step is carried out by the truncated addition operation, with the new rank k determined based on the accuracy requirement ε_{opt}. To validate the effectiveness of the proposed $\mathcal{H}$-partition optimization algorithm, we simulated a conducting plate from 2λ to 60 λ with unknowns from 1,160 to 1,078,800. The ε_{opt} was chosen as 10^{-3}. In Fig. 2, we plot the maximum number of admissible blocks that can be formed by one cluster in a block cluster tree (C_{ad}) in the original $\mathcal{H}$ partition, and that in the optimized $\mathcal{H}$ partition. Clearly, the C_{ad} is reduced greatly. Since the proposed $\mathcal{H}$-partition optimization does not increase the number of inadmissible blocks, the C_{sp} is also reduced significantly.

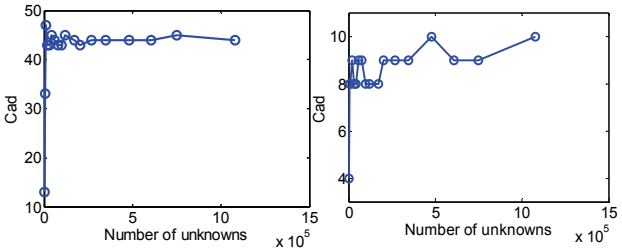

Fig. 2 C_{ad} versus N in the simulation of a PEC plate (a) Original $\mathcal{H}$-partition. (b) Optimized $\mathcal{H}$-partition.

C. Fast LU-based direct solution. Based on the schemes above, we develop a fast LU factorization with $O(k_{ave}^2 C_{sp}^2 N\log^2 N)$ time complexity and $O(k_{\text{ave}}C_{\text{sp}}N\log N)$ memory complexity using the $\mathcal{H}$-based representation of **G** and **G**'s LU factors, with k_{ave} and C_{sp} minimized to be negligible compared to N. We develop a number of pseudo-codes to perform a fast implementation of the $\mathcal{H}$-based LU factorization, which are omitted here due to space limit.

Numerical Results

The *leafsize* = 32 was used in all simulations. The error tolerance used in the $\mathcal{H}$-partition optimization and LU factorization was set as 10^{-3} and 10^{-2}, respectively. The computer used

was a Dell's PowerEdge 6950s server with an 8222SE AMD Opteron processor. The first example is a conducting sphere with electric size from 2λ to 26λ having unknowns from 3,688 to 636,840. Fig. 3 shows the average rank k_{ave} resulting from the proposed schemes. It can be seen that k_{ave} is minimized to be a small number compared to N. To test the accuracy, we plot the E-plane bi-static RCS simulated for 26λ in Fig. 5(a), which is shown to agree well with the analytical Mie-Series solution. In Fig. 5(b) and (c), we plot the memory and time complexity of the proposed LU-based direct solver. The theoretical complexity is also plotted for comparison. Excellent agreement is observed. The second example is a 3D conducting plate with electric size from 2λ to 60λ, and unknowns from 1,160 to 1,078,800. The average rank k_{ave} is shown in Fig. 4. The accuracy of the proposed solver is controlled to be almost a constant in the entire range of electric sizes as can be seen from Fig. 6(a). In Fig. 6(b) and (c), we plot the memory and time complexity of the proposed direct IE solver, which agree well with the theoretical complexity depicted by the solid lines. It can be seen that the computation for the 60λ case having over 1 million unknowns was finished within 10-hour LU decomposition time, 55-second LU solution time, and costing 31.5 GB storage only. We also simulated a cylinder of length from 2 λ to 96 λ. The ratio of length to radius is 20. The number of unknowns is from 1,391 to 1,075,200. The LU factorization for the 1,075,200 unknown case costs less than 20 hours and 37.6 GB memory. The LU solution time is 85 seconds only. Double precision was used in all simulations.

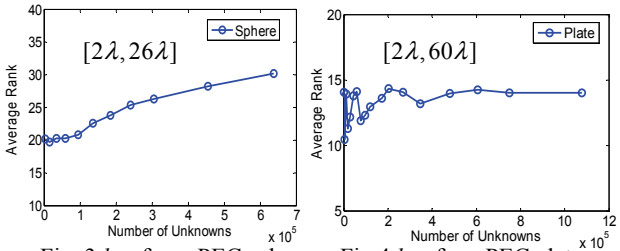

Fig. 3 k_{ave} for a PEC sphere

Fig.4 k_{ave} for a PEC plate

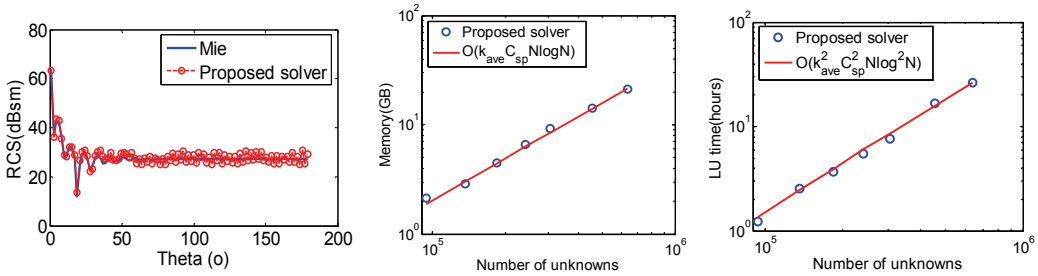

Fig. 5 Simulation of a PEC sphere. (a) RCS. (b) Memory. (c) LU factorization time.

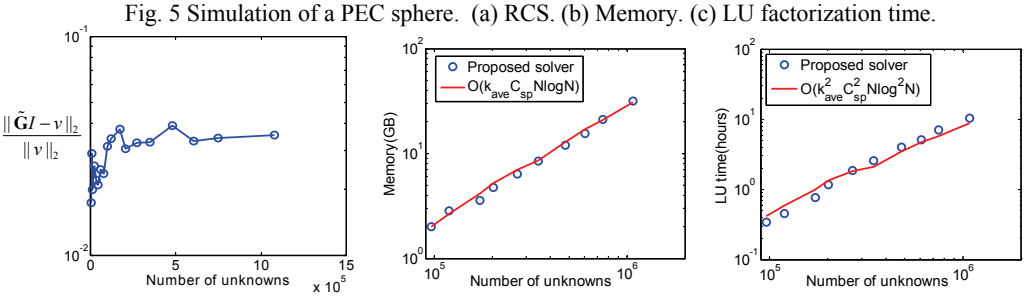

Fig. 6 Simulation of a PEC plate. (a) Solution error. (b) Memory. (c) LU factorization.

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