

# $O(N)$ Iterative and $O(N\log N)$ Direct Volume Integral Equation Solvers for Large-Scale Electrodynamical Analysis

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**Abstract** — State-of-the-art volume integral equation (VIE) solvers for solving electrically large problems are iterative solvers with the complexity of each matrix-vector multiplication being  $O(N\log N)$ , where  $N$  is matrix size. In this work, we reduce this complexity to strictly  $O(N)$  irrespective of electrical size. Furthermore, we develop a fast inversion based direct VIE solver of  $O(N\log N)$  complexity, which is also independent of electrical size. Numerical experiments have demonstrated the complexity, accuracy, and efficiency of the proposed new VIE solvers. Very large-scale VIE system matrices involving millions of unknowns have been directly solved in fast CPU time and modest memory consumption on a single core running at 3 GHz.

## 1 Introduction

Driven by the design of advanced engineering systems, there is a continued need for reducing the complexity of computational electromagnetic (EM) methods. Among these methods, the volume integral equation (VIE) based methods have a great flexibility in modeling both complicated geometry and inhomogeneous materials in open-region settings. Existing fast VIE solvers for solving large-scale problems are, in general, iterative solvers which rely on efficient matrix-vector multiplications. The complexity of one matrix-vector multiplication in a VIE solver has been significantly reduced from  $O(N^2)$  to  $O(N\log N)$  for analyzing electrodynamic problems.

In this work, we represent the dense system matrix resulting from the volume integral equation based analysis of general electromagnetic problems by an  $\mathcal{H}^2$ -matrix [1] with controlled accuracy. We develop an efficient algorithm to generate such an  $\mathcal{H}^2$ -matrix representation with the rank of each admissible block minimized based on prescribed accuracy. The resultant rank hence scales linearly with the electrical size of the admissible block instead of cubically in a general 3-D problem. With the rank's growth with electrical size taken into account, we

developed linear-complexity  $\mathcal{H}^2$ -matrix-based storage and matrix-vector multiplication, and thereby an  $O(N)$  iterative VIE solver regardless of electrical size. Moreover, we developed an  $O(N\log N)$  matrix inversion, and hence a fast  $O(N\log N)$  direct VIE solver for large-scale electrodynamic analysis.

## 2 Minimal-Rank Representation of the VIE Operator and the Resultant Rank's Growth with Electrical Size

Unlike static problems, the rank of an electrodynamic IE kernel increases with electrical size for achieving a prescribed accuracy, which results in a higher computational complexity if no advanced algorithms are conceived to effectively manage the rank's growth with electrical size. The true indicator of this rank's growth is singular value decomposition (SVD), since its resultant representation constitutes a minimal rank representation of a matrix for any prescribed accuracy. The SVD does not separate sources from observers in approximating Green's function, and it finds a minimal rank representation of the IE kernel as a whole. The SVD is computationally  $O(N^3)$ , and hence not practically feasible for studying the rank of electrically large IE operators. In view of the pivotal importance of this subject, a theoretical study has been carried out on the rank's growth with electrical size in integral equations [2]. The significance of this study lies in the fact that it derives a closed-form analytical expression of the rank of the coupling Green's function, which has the same scaling as that depicted by SVD-based rank revealing. The findings on the rank-study are summarized as follows:

- 1) The rank ( $k$ ) of the off-diagonal block, irrespective of the electrical size, is far less than the size of the block, thus the off-diagonal block has a low rank representation, i.e.  $k \ll N$ .
- 2) For static and one-dimensional configurations of sources and observers, the rank required by a prescribed accuracy remains constant irrespective of the problem size.
- 3) For 2- and 3-D configurations, the rank varies as square root of logarithm and linearly with the electrical size, respectively.

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The above findings have also been numerically verified by realistic VIE examples given in Section 5.

### 3 Algorithm For Generating a Minimal-Rank $\mathcal{H}^2$ -Representation

An  $\mathcal{H}^2$ -representation is a nested low-rank representation [1] of a dense matrix. To generate such a representation, if we separate sources  $\vec{r}$  from observers  $\vec{r}$  in approximating Green's function, the resultant rank is a full rank in order to represent a function of complete  $\vec{r}$  or  $\vec{r}$ . We hence cannot use source-observer separated methods to generate an  $\mathcal{H}^2$ -representation whose rank is *minimal* for the prescribed accuracy. In this work, we propose to start from an algebraic  $\mathcal{H}$ -representation [3] of the VIE system matrix, and then convert it to a nested  $\mathcal{H}^2$ -representation with minimal rank. The numerical procedure is a bottom-up traversal of the cluster tree as follows.

For each leaf cluster  $t$ , we construct a Gram matrix  $\mathbf{G}_2^t$  as the following.

$$\mathbf{G}_2^t = \mathbf{G}^{(t,s)} \mathbf{G}^{(t,s)\mathbf{H}} = \sum_{i \in \text{self-level}} \mathbf{A}_i (\mathbf{B}_i^T \bar{\mathbf{B}}_i) \mathbf{A}_i^{\mathbf{H}} + \sum_{i \in \text{ancestor-level}} \mathbf{A}_i^t (\mathbf{B}_i^T \bar{\mathbf{B}}_i) \mathbf{A}_i^{\mathbf{H}} \quad (1)$$

In the above,  $\bar{\mathbf{B}}_i$  is the complex conjugate of  $\mathbf{B}_i$ , and  $\mathbf{B}_i^T \bar{\mathbf{B}}_i$  is a  $k \times k$  matrix, prepared a-priori for each of the admissible block, and then used to construct  $\mathbf{G}_2^t$ .  $\mathbf{A}_i^t$ , in the second summation term above, is nothing but the sub-block corresponding to row cluster  $t$  of the bigger matrix  $\mathbf{A}$  at any ancestral level. After generating  $\mathbf{G}_2^t$ , we perform an accuracy-controlled Schur/SVD decomposition of (1) such that  $\mathbf{G}_2^t = \mathbf{PDP}^{\mathbf{H}}$  to get the new leaf cluster basis as  $\mathbf{V}^t = \mathbf{P}$ . Since each  $\mathbf{G}_2^t$  is of *leafsize*, this can be done efficiently.

For each non-leaf cluster  $t$ , since we have already determined the lower level cluster bases and dare not to operate on  $O(N^2)$  Gram matrices, we form their projected form, which is analytically built by projecting the Gram matrix onto its children's cluster bases to get an  $O(k^2)$  matrix  $\mathbf{G}_{2,\text{proj}}^t$ . The reason for this is to perform an SVD of an  $O(k^2)$  matrix at every tree level  $l$  instead of a  $\#t \times \#t$  matrix of (1).

$$\mathbf{G}_{2,\text{proj}}^t = \sum_{i \in \text{self}} \mathbf{A}_{i\text{small}} (\mathbf{B}_i^T \bar{\mathbf{B}}_i) \mathbf{A}_{i\text{small}}^{\mathbf{H}} + \sum_{i \in \text{ancestors}} \mathbf{A}_{i\text{small}}^t (\mathbf{B}_i^T \bar{\mathbf{B}}_i) \mathbf{A}_{i\text{small}}^{\mathbf{H}} \quad (2)$$

where,  $\mathbf{A}_{i\text{small}} = \begin{bmatrix} \mathbf{V}^{t1} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^{t2} \end{bmatrix}^{\mathbf{H}} \mathbf{A}_i$  and each of this multiplication evaluation costs  $O(k^2(\#t))$  and requires only  $O(k^2)$  storage units. The remaining multiplications involve three  $O(k^2)$ -sized matrices requiring total complexity of  $O(k^3)$  operations. Then we perform an SVD of the small sized  $\mathbf{G}_{2,\text{proj}}^t$  to obtain  $\mathbf{G}_2^t = \mathbf{PDP}^{\mathbf{H}}$  based on the prescribed accuracy. The transfer matrices of the new cluster basis at this non-leaf level is nothing but  $\begin{bmatrix} \mathbf{E}^{t1} \\ \mathbf{E}^{t2} \end{bmatrix} = \begin{bmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \end{bmatrix}$ . After the rank-minimized nested cluster bases have been generated, the coupling matrices are updated based on the new cluster bases.

### 4 $O(N)$ Storage and Matrix-Vector Multiplication and $O(N \log N)$ Matrix Inversion

In a VIE, the electrical size scales  $O(N^{\frac{1}{3}})$ , and hence the rank  $k$  of a minimal-rank representation scales as  $O(N^{\frac{1}{3}})$ . With such a rank's dependence on  $N$ , the memory complexity of an  $\mathcal{H}^2$ -matrix can be analyzed as the following, which is also the complexity of one matrix-vector multiplication:

$$\begin{aligned} \text{Comp}(\text{Memory/MVM}) &= O\left(\sum_{l=0}^L \left(\frac{N}{2^l}\right)^{\frac{2}{3}} C_{sp} 2^l\right) \\ &= O\left(C_{sp} N^{\frac{2}{3}} \sum_{l=0}^L 2^{\frac{l}{3}}\right) = O(N). \end{aligned} \quad (3)$$

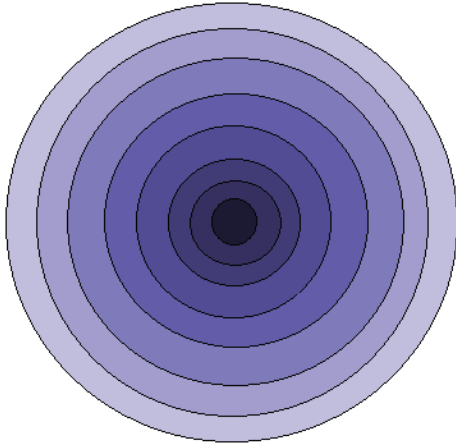
For matrix inversion, we have the following complexity

$$\begin{aligned} \text{Comp}(\text{Inversion}) &= O\left(\sum_{l=0}^L \left(\frac{N}{2^l}\right)^{\frac{3}{3}} C_{sp}^2 2^l\right) \\ &= O\left(C_{sp}^2 N \sum_{l=0}^L 1\right) = O(N \log N). \end{aligned} \quad (4)$$

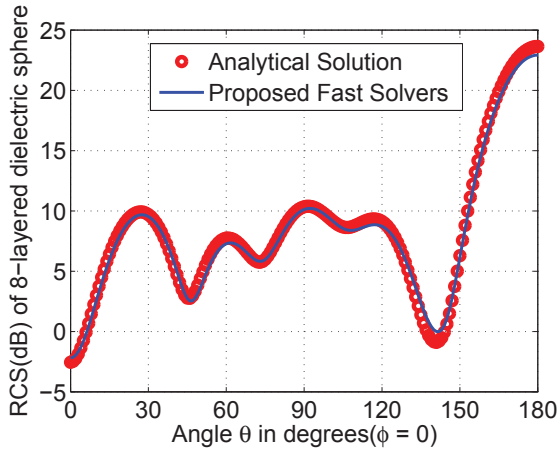
Thus we see that for a VIE, as soon as an  $\mathcal{H}^2$ -matrix with a minimal-rank representation is used, the underlying storage and matrix-vector multiplication cost becomes linear while the inversion cost becomes as fast as  $O(N \log N)$ , regardless of electrical size.

### 5 Numerical Results

The first example is an 8-layer dielectric sphere where the dielectric constant from inner-most to outer-most layer decreases in step of 0.5 from 5.0 to 1.5. The structural detail is depicted in Fig. 1(a). The RCS comparison with analytical Mie-series solution can be seen in Fig. 1(b).



(a) Multilayer dielectric sphere.



(b) RCS comparison with Mie-series solution.

Figure 1: Multilayer dielectric sphere of  $k_0a = 6.28$ : structure and RCS comparison.

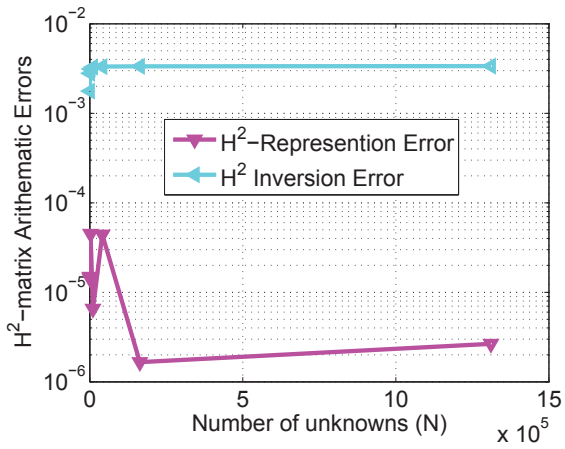
Next, we simulate a dielectric rod of square cross-section of dimensions  $\lambda_0/10 \times \lambda_0/10$ , while its length is kept on increasing from  $\lambda_0$  to  $8192\lambda_0$  at 300 MHz. This results in the scaling of number of unknowns from as small as 162 to as large as 1.31 million. The dielectric constant is 2.54. Each of these structures is illuminated by an incident plane wave  $\vec{E}^i(\vec{r}) = e^{jk_0y}\hat{z}$ . In Fig. 2(a), the representation and inversion accuracy is shown as a function of  $N$ . The accuracy of the inverse is well-controlled below 0.5% error for the whole electrical size range. As evident from Fig. 2(b), the accuracy determined rank remains to be constant throughout the range of electrical size being simulated, which agrees well with that analytically derived in [2]. The total number of iterations for this example also remains constant  $N_{it} = 5$  for a convergence criterion of  $10^{-3}$  using BiCGStab iterative solver. In Fig. 2(c),

the scaling of the computational resources with the number of unknowns is shown to be linear both for the iterative as well as the direct solver. Even for a dense matrix of 1.31 million unknowns, it only takes around 40 mins to get an accuracy controlled inverse of the VIE system matrix. The iterative solver, on the other hand, gives the solution in less than 4 mins for one right hand side.

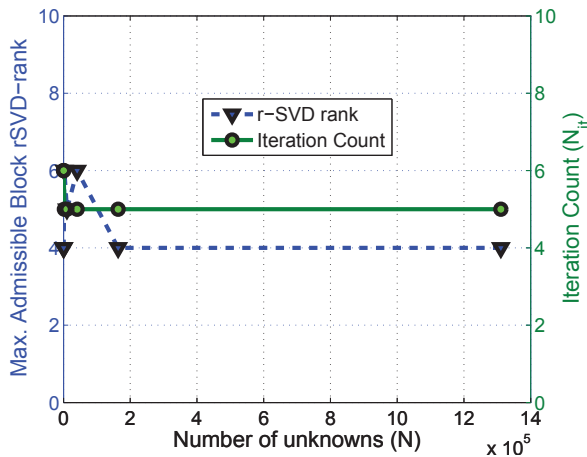
Next, we simulate a large-scale array of dielectric cubes of size  $0.3\lambda_0 \times 0.3\lambda_0 \times 0.3\lambda_0$  at 300 MHz. The distance between the neighboring cubes is kept to be  $0.3\lambda_0$ . The number of these cubes is increased in each of the  $x$ -,  $y$ - and  $z$ - directions, resulting in  $2 \times 2 \times 2$  then  $4 \times 4 \times 4$ , and finally to  $8 \times 8 \times 8$  cubes. This results in the scaling of number of unknowns from 3024 to 193,536. The dielectric constant in each cube is 4.0. This structure is illuminated by an incident plane wave  $\vec{E}^i(\vec{r}) = e^{jk_0y}\hat{z}$ . In Fig. 3(a), the representation and inversion accuracy is shown as a function of  $N$ . The accuracy of the inverse is well-controlled below 5% error for the whole electrical size range. The rank of the off-diagonal blocks is also found to increase linearly with the electrical size of the problem, which confirms the theoretical finding in [2]. In Fig. 3(b), the scaling of the computational resources with the number of unknowns is shown. It can be observed that for smaller number of unknowns, the scaling is not linear. The core reason for this is because for this unknown range, in a 3-D setting, the sparsity constant ( $C_{sp}$ ) has not become constant and still fluctuates from one level to another. As soon as it saturates, we can observe linear scaling of memory and matrix-vector multiplication costs. For the direct inverse, again we observe an  $O(N \log N)$  scaling in Fig. 3(c) for the last three points where the  $C_{sp}$  has become saturated.

## References

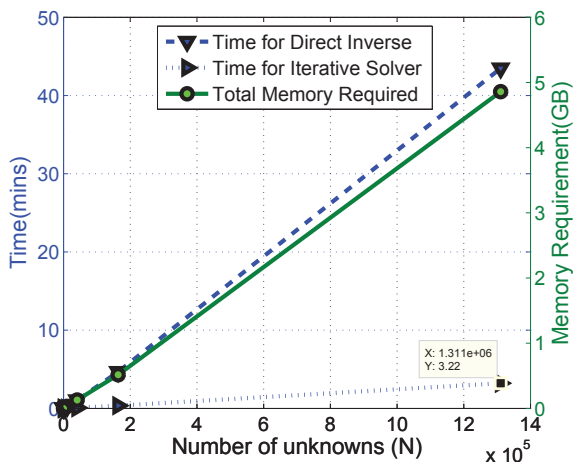
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- [3] W. Chai and D. Jiao, "A complexity-reduced H-matrix based direct integral equation solver with prescribed accuracy for large-scale electrodynamic analysis," in *Proc. IEEE Int. Symp. Antennas Propag.*, 4 pages, Jul. 2010.



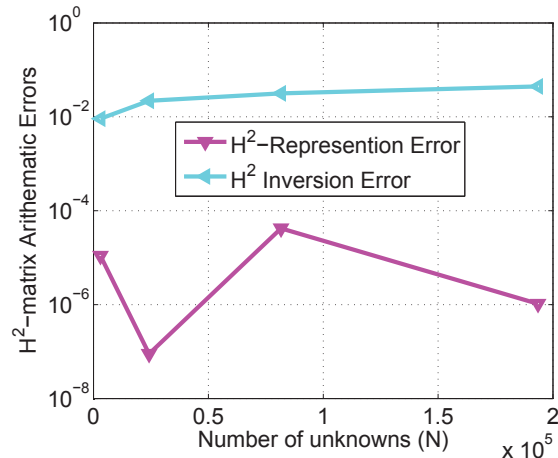
(a)  $\mathcal{H}^2$ -matrix representation and inversion accuracy.



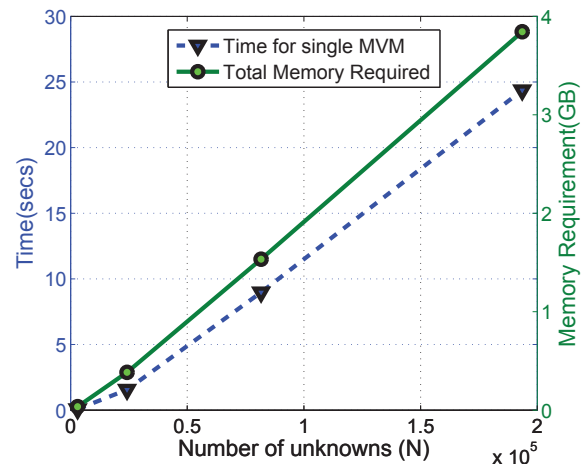
(b) Rank and iteration counts.



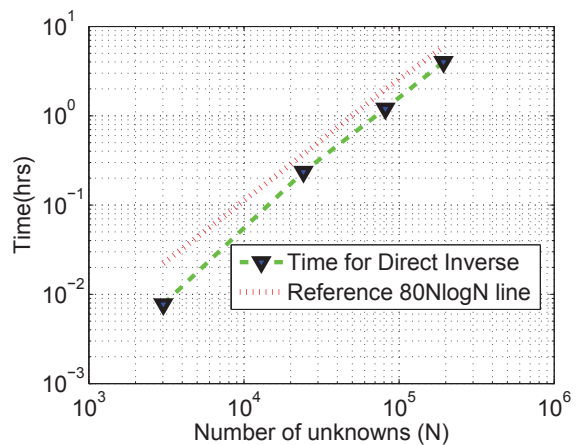
(c) Time and memory complexity.



(a)  $\mathcal{H}^2$ -matrix representation and inversion accuracy.



(b) Scaling of memory and single MVM cost.



(c) Scaling of inversion time.

Figure 2: Dielectric rod: Performance of proposed fast VIE solvers as a function of  $N$ .

Figure 3: Dielectric cube array: Performance of the proposed iterative and direct VIE solvers.