# A Butterfly-Accelerated Volume Integral Equation Solver for Broad Permittivity and Large-Scale Electromagnetic Analysis 

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#### Abstract

A butterfly-accelerated volume integral equation (VIE) solver is proposed for fast and accurate electromagnetic (EM) analysis of scattering from heterogeneous objects. The proposed solver leverages the hierarchical off-diagonal butterfly (HOD-BF) scheme to construct the system matrix and obtain its approximate inverse, used as a preconditioner. Complexity analysis and numerical experiments validate the $O\left(N \log ^{2} N\right)$ construction cost of the HOD-BF-compressed system matrix and $O\left(N^{1.5} \log N\right)$ inversion cost for the preconditioner, where $N$ is the number of unknowns in the high-frequency $E M$ scattering problem. For many practical scenarios, the proposed VIE solver requires less memory and computational time to construct the system matrix and obtain its approximate inverse compared to a $\mathcal{H}$ matrix-accelerated VIE solver. The accuracy and efficiency of the proposed solver have been demonstrated via its application to the EM analysis of large-scale canonical and real-world structures comprising of broad permittivity values and involving millions of unknowns.


Index Terms-Butterfly algorithm, direct solver, fast solver, preconditioners, volume integral equation.

## I. INTRODUCTION

THE analysis of electromagnetic (EM) scattering from heterogeneous scatterers is traditionally performed via volume integral equation (VIE) solvers [1]-[3]. These solvers discretize the VIE and obtain a dense system of linear equations with $N$ unknowns. Oftentimes, these solvers' applicability to the large-scale problems is limited due to $O\left(N^{2}\right)$ or $O\left(N^{3}\right)$ memory and CPU time requirements for the iterative or direct solution of the dense VIE system, respectively. On the other hand, differential equation solvers require the solution of a sparse system of linear equations and consequently demand less computational resources compared to VIE solvers when applied to the large-scale problems. That said, unlike VIE solvers, differential equation solvers do not implicitly satisfy the radiation conditions and can suffer from the numerical dispersion.

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So far, a plethora of methods has been developed to lower the memory and CPU time requirements of VIE solvers [4][12]. These methods were primarily developed to expedite the matrix-vector multiplications during the iterative solution of the VIE system. They leverage analytic or algebraic compression techniques, including the fast multipole method (FMM) [4], [5], fast Fourier transform [6]-[8], [13], low-rank compression [9], hierarchical matrices as kernel-free FMM [10], [11], and, more recently, tensor decompositions [12]. Despite the success of these methods in expediting matrixvector multiplications during iterative solution, the discretized VIE systems are often ill-conditioned. This results in a prohibitively large iteration count during the iterative solutions of the VIE systems. In particular, the systems are ill-conditioned in scenarios where the scatterers have large permittivity [14][18], negative permittivity [19]-[22], or large electrical size. This results in several challenges for using VIE in the EM analysis of biomedical procedures applied to high-permittivity tissues [23], EM analysis of the structures covered by negative permittivity plasma [24], and EM analysis of electrically-large photonic devices [25]. For these scenarios, fast matrix-vector multiplication schemes have to be used in conjunction with effective preconditioners. Alternatively, fast direct methods can be utilized.

Existing fast direct solvers for the VIE include Huygens' equivalence principle-based algorithms [26], [27] yielding an $O\left(N^{2}\right)$ complexity, and low-rank-based algorithms such as $\mathcal{H}$ matrices [28], [29], $\mathcal{H}^{2}$ matrices [30]-[32], and skeletonization [20], [33], [34]. These low-rank-based algorithms can attain $O(N)$ or $O(N \log N)$ complexities for static or low-frequency scattering problems, but tend to become less efficient as the electrical size of the scatterer increases. Low-rank-based direct solvers have also been developed for surface integral equations (SIE) [10], [11], [35], but low-rank algorithms tend to perform better for VIE solvers. This is due to the fact that the density of discretization elements per wavelength is typically much larger for the VIE compared to that for the SIE.

In contrast to the low-rank algorithms, here we consider another class of algebraic compression techniques called butterfly algorithms [36]-[40] for fast iterative and/or direct solution of the VIE. For a $m \times n$ matrix, its butterfly representation can be treated as an extension of the fast Fourier transform into an $O(\log n)$-factor multiplicative matrix decomposition that is well-suited to compress highly-oscillatory operators [41][43]. Each butterfly factor contains $O(n)$ number of small
dense blocks whose sizes are oftentimes referred to as butterfly ranks. When combined with hierarchical matrix techniques, they have been leveraged for the direct or iterative solutions of 2-dimensional [37], [44]-[46], 3-dimensional [47]-[49] SIE, and differential equations [50] for electrically-large scattering problems. In general, the butterfly-accelerated SIE solvers can be classified into the strong-admissibility condition-based ones (such as hierarchical LU [47]) and weak-admissibility conditioned-based ones (such as hierarchically off-diagonal butterfly (HOD-BF) algorithm [45]). The former compresses only matrix blocks for the well-separated interactions, while the latter compresses the matrix blocks for both nearby and well-separated interactions [51]. They can be treated as the butterfly extensions of the strong-admissibility $\mathcal{H}$ [28] and weak-admissibility hierarchically off-diagonal low-rank (HOD-LR) [52]-[54] matrices, respectively.

This paper proposes a butterfly-accelerated VIE solver for the EM scattering analyses of large-scale scatterers comprising broad permittivity values. The proposed solver leverages the HOD-BF scheme to compress the blocks in the VIE system and obtain the approximate inverse of the system matrix for forming a preconditioner. During the iterative solution of the VIE system, the matrix-vector multiplications are accelerated using the HOD-BF-compressed blocks while the iteration count is dramatically dropped to single digits with the preconditioner, even for highly ill-conditioned problems. Compared to the strong-admissibility solvers [47], [48], the proposed solver has simpler butterfly arithmetic, smaller leading constants in complexity, and significantly better parallelization performance. The HOD-BF scheme leveraged in the proposed solver was first introduced as a sequential algorithm to solve 2-dimensional SIE with $O\left(N \log ^{2} N\right)$ memory and $O\left(N^{1.5} \log N\right)$ CPU time requirements [45]; the same complexity can also be attained for 3-dimensional SIE despite of the non-uniform rank patterns due to weak-admissibility [55]. To the best of our knowledge, neither the HOD-BF scheme nor other butterfly schemes has been applied to the 3-dimensional VIE before, and consequently the complexity analysis of HOD-BF scheme has never been performed for the VIE. Unlike the HOD-LR scheme that scales poorly for high-dimensional problems, e.g., $O\left(N^{5 / 3}\right)$ memory and $O\left(N^{7 / 3}\right)$ CPU for 3D VIEs, we show that HOD-BF scheme's complexity is dimension independent. Furthermore, the advantages of the HOD-BF scheme compared to the low-rankbased $\mathcal{H}$ matrix scheme have never been shown. All the numerical experiments are carried out using a distributedmemory parallel implementation of HOD-BF, briefly explained in this study. Without such implementation, the demonstration of the advantages of HOD-BF compared to the HOD-LR and $\mathcal{H}$ matrix schemes would not be possible. These are the novelties introduced in this paper.

Here, we theoretically and numerically analyze the rank scaling and complexity of the proposed HOD-BF-accelerated VIE solver. Furthermore, we extensively compare the performance of the proposed VIE solver with that of a low-rank-based $\mathcal{H}$ matrix-accelerated VIE solver. The numerical analysis shows that the proposed solver achieves $O\left(N \log ^{2} N\right)$ memory and CPU time scaling for constructing the HOD-BF-
compressed system matrix as well as $O\left(N \log ^{2} N\right)$ memory and $O\left(N^{1.5} \log N\right)$ CPU time scaling for inverting the system matrix to obtain the preconditioner. Compared to the $\mathcal{H}$ matrixaccelerated VIE solver, the proposed solver requires 1.4/3.5 times less CPU time and 3.8/3.9 times less memory for the construction/inversion when used for the EM analysis of a dielectric sphere involving 0.9 M unknowns. Similar comparison performed on a NASA almond involving 1.6 M unknowns shows that the proposed simulator requires 5.0/3.2 times less CPU time and 3.8/2.7 times less memory for the construction/inversion compared to the $\mathcal{H}$ matrix-accelerated VIE solver. Moreover, the proposed solver with the preconditioner requires maximum five iterations during the iterative solution of an highly ill-conditioned VIE system generated for the EM scattering analysis of negative permittivity sphere involving 1.7 M unknowns.

The rest of the paper is organized as follows: Section II describes the VIE formulation. Section III presents the construction of the HOD-BF-compressed system matrix via butterfly algorithm, inversion of the compressed system matrix to obtain preconditioner, complexity estimates, and parallelization strategy. Section IV provides numerical results to demonstrate the scalability, accuracy, and efficiency of the proposed butterflyaccelerated VIE solver. The conclusions are drawn in Section V. Throughout this paper, a time-harmonic variation of field quantities is assumed and suppressed.

## II. VIE Formulation

Consider a time-harmonic EM field with incident electric and magnetic fields, $\mathbf{E}^{\text {inc }}(\mathbf{r})$ and $\mathbf{H}^{\text {inc }}(\mathbf{r})$, at frequency $f$. The field impinges on a heterogeneous scatterer $V$ residing in a background medium with permittivity $\varepsilon_{0}$, permeability $\mu_{0}$, and intrinsic impedance $\eta_{0}=\sqrt{\mu_{0} / \varepsilon_{0}}$. Here the background medium is assumed to be free-space. Using the volume equivalence principle, the VIE for the electric flux density $\mathbf{D}(\mathbf{r})$ is obtained as [1]

$$
\begin{equation*}
\mathbf{D}(\mathbf{r}) / \varepsilon(\mathbf{r})-j \omega \eta_{0} \mathcal{L}[\kappa \mathbf{D}](\mathbf{r})=\mathbf{E}^{\mathrm{inc}}(\mathbf{r}) ; \mathbf{r} \in V \tag{1}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathcal{L}[\mathbf{X}](\mathbf{r})=-j k_{0} \int_{V} d v^{\prime}\left[\mathbf{I}+\frac{1}{k_{0}^{2}} \nabla \nabla \cdot\right] \mathbf{X}(\mathbf{r}) \mathbf{g}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \tag{2}
\end{equation*}
$$

Here $\omega=2 \pi f$ is the angular frequency, $\mathbf{r}$ and $\mathbf{r}^{\prime}$ are the observation and source points, $k_{0}=\omega \sqrt{\mu_{0} \varepsilon_{0}}=2 \pi / \lambda_{0}$ is the wave number, $\lambda_{0}$ is the wavelength, $\varepsilon(\mathbf{r})$ is the dielectric permittivity, $\kappa(\mathbf{r})=\left(\varepsilon(\mathbf{r})-\varepsilon_{0}\right) / \varepsilon(\mathbf{r})$ is the dielectric contrast, and $\mathbf{g}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=e^{-j k_{0}\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} / 4 \pi\left|\mathbf{r}-\mathbf{r}^{\prime}\right|$ is the Green's function.

To solve the VIE, the scatterer is discretized by a volumetric tetrahedral mesh having $N$ faces. Then, the electric flux in $V$ is approximated via Schaubert Wilton Glisson (SWG) basis functions $\mathbf{f}_{n}(\mathbf{r})$ as [1]

$$
\begin{equation*}
\mathbf{D}(\mathbf{r})=\sum_{n=1}^{N} D_{n} \mathbf{f}_{n}(\mathbf{r}) ; \mathbf{r} \in V \tag{3}
\end{equation*}
$$

Note that one SWG is defined for each of the $N$ faces of the tetrahedral mesh, and each basis function $\mathbf{f}_{n}(\mathbf{r})$ has support on $V_{n}$, the volume of the tetrahedron which the face $N$ belongs to.

Substituting (3) into (1) and applying Galerkin testing yields the discretized VIE linear system of equations as

$$
\begin{equation*}
\mathcal{Z I}=\mathcal{V} \tag{4}
\end{equation*}
$$

where

$$
\begin{align*}
\mathcal{Z}(m, n) & =\left\langle\mathbf{f}_{m}(\mathbf{r}), \frac{\mathbf{f}_{n}(\mathbf{r})}{\varepsilon(\mathbf{r})}-j \omega \eta \mathcal{L}\left(\kappa(\mathbf{r}) \mathbf{f}_{n}(\mathbf{r})\right)\right\rangle_{m} \\
\mathcal{I}(n) & =D_{n} \\
\mathcal{V}(m) & =\left\langle\mathbf{f}_{m}(\mathbf{r}), \mathbf{E}^{\operatorname{inc}(\mathbf{r})}\right\rangle_{m} ; \quad n, m=1, \ldots, N \tag{5}
\end{align*}
$$

Here, $\mathcal{Z}$ is the system matrix, $\mathcal{I}$ is the unknown coefficient vector, and $\mathcal{V}$ is the excitation vector. Furthermore, $\kappa(\mathbf{r})=$ $\left(\varepsilon(\mathbf{r})-\varepsilon_{0}\right) / \varepsilon(\mathbf{r})$ and $<\mathbf{a}, \mathbf{b}>_{m}=\int_{V_{m}} \mathbf{a} \cdot \mathbf{b} d \mathbf{r}$ denotes the standard inner product of a with $\mathbf{b}$ in $V_{m}$.

The linear system (4) is solved with preconditioned iterative solvers as

$$
\begin{equation*}
\mathcal{Z}_{\chi_{\text {fact }}}^{-1} \mathcal{Z}_{\chi_{c o n}} \mathcal{I}=\mathcal{Z}_{\chi_{\text {fact }}}^{-1} \mathcal{V} \tag{6}
\end{equation*}
$$

Here $\mathcal{Z}_{\chi_{c o n}}$ is a compressed representation of $\mathcal{Z}$ with tolerance $\chi_{c o n}$ using e.g., $\mathcal{H}$ [28], HOD-LR [52], or the proposed HODBF [45] techniques. $\mathcal{Z}_{\chi_{\text {fact }}}^{-1}$ is the compressed representation of $\mathcal{Z}^{-1}$ with tolerance $\chi_{\text {fact }} \geq \chi_{\text {con }}$. We will drop the subscripts of $\mathcal{Z}_{\chi_{c o n}}$ and $\mathcal{Z}_{\chi_{f a c t}}^{-1}$ in the rest of this paper. The preconditioned linear system (6) can be solved via an iterative solver (such as the transpose-free quasi-minimal residual method (TFQMR) [56]) by setting a stopping criteria $\chi_{\text {sol }}$.

## III. HOD-BF Acceleration and Preconditioner

The HOD-BF scheme first generates a hierarchical partitioning of the system matrix and then obtains the compressed off-diagonal blocks representing non-overlapping interactions as the butterfly format. The compressed blocks permit rapid matrix-vector multiplications and inversion, particularly for high-frequency regimes and 3-dimensional scatterers. In what follows, we briefly summarize the construction of the system matrix via HOD-BF-compressed blocks and inversion of the compressed system matrix to obtain preconditioner.

## A. Construction of HOD-BF-compressed system matrix

The construction begins by recursively subdividing the scatterer into two sub-scatterers with approximately equal numbers of unknowns using a tree clustering algorithm (such as KD) [44], until the subscatterer contains a prescribed number of unknowns. This procedure results in a complete binary tree $\mathfrak{T}_{H}$ of $L_{H}$ levels with root level 0 and leaf level $L_{H}$. Each node $\tau$ at level $l$ is an index set $\tau \subset\{1, \ldots, N\}$ associated with the corresponding subscatterer. For a non-leaf node $\tau$ at level $l$ with children $\tau_{1}$ and $\tau_{2}, \tau=\tau_{1} \cup \tau_{2}$ and $\tau_{1} \cap \tau_{2}=\emptyset$. For a non-root node $\tau$, its parent is denoted $p_{\tau}$. Let $\mathcal{D}_{\tau}=\mathcal{Z}(\tau, \tau)$. For the root $\tau, \mathcal{D}_{\tau}=\mathcal{Z}$; for each leaf node $\tau, \mathcal{D}_{\tau}$ is directly computed as dense blocks; off-diagonal blocks are compressed using the butterfly representation described below. As an example, Fig. 1 shows a HOD-BF-compressed matrix with $L_{H}=3$ levels.

Specifically, let $\tau_{1}$ and $\tau_{2}$ be two siblings in $\mathfrak{T}_{H}$ on level $l$. These two sibling nodes correspond to two off-diagonal
blocks $\mathcal{B}_{\tau_{1}}=\mathcal{Z}\left(\tau_{1}, \tau_{2}\right)$ and $\mathcal{B}_{\tau_{2}}=\mathcal{Z}\left(\tau_{2}, \tau_{1}\right)$. As an example consider the butterfly compression of the $m \times n$ block $\mathcal{B}=\mathcal{B}_{\tau_{1}}$ with $o=\tau_{1}$ and $s=\tau_{2}$, then $\mathcal{B}=\mathcal{Z}(o, s)$ is compressed as a butterfly with $L=L_{H}-l$ levels. Let $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$ denote subtrees of $\mathfrak{T}_{H}$ with $L$ levels, rooted at nodes $o$ and $s$ respectively. The butterfly compression requires the complementary low-rank property: for any level $0 \leq l \leq L$, any node $\tau$ at level $l$ of $\mathfrak{T}_{o}$ and any node $\nu$ at level $L-l$ of $\mathfrak{T}_{s}$, the subblock $\mathcal{Z}(\tau, \nu)$ is numerically low-rank with rank $r_{\tau, \nu}$ bounded by a small number $r$ called the butterfly rank. As will be discussed in Section III-C, we do not necessarily require constant butterfly ranks to attain a quasi-linear representation. Given the complementary low-rank property, we can compress any subblock $\mathcal{Z}(\tau, \nu)$ above as a low-rank product in an interpolative form:

$$
\begin{equation*}
\mathcal{Z}(\tau, \nu) \approx \mathcal{Z}(\tau, \bar{\nu}) \mathcal{V}_{\tau, \nu} \tag{7}
\end{equation*}
$$

where $\bar{\nu}$ represents the skeleton columns, $\mathcal{Z}(\tau, \bar{\nu})$ is the skeleton matrix, and $\mathcal{V}_{\tau, \nu}$ is the interpolation matrix. The approximation in Eq. (7) is typically computed with a compression tolerance $\chi_{c o n}$ such that $\left|\mathcal{Z}(\tau, \nu)-\mathcal{Z}(\tau, \bar{\nu}) \mathcal{V}_{\tau, \nu}\right|_{F}=$ $O\left(\chi_{c o n}\right)|\mathcal{Z}(\tau, \nu)|_{F}$. This low-rank product can be computed from the interpolative decomposition (ID) [57]. Moreover, the interpolation matrices $\mathcal{V}_{\tau, \nu}$ for non-leaf nodes $\nu$ can be defined in a nested fashion as

$$
\mathcal{V}_{\tau, \nu}=\mathcal{W}_{\tau, \nu}\left[\begin{array}{ll}
\mathcal{V}_{p_{\tau}, \nu_{1}} &  \tag{8}\\
& \mathcal{V}_{p_{\tau}, \nu_{2}}
\end{array}\right]
$$

where $\mathcal{W}_{\tau, \nu}$ are referred to as the transfer matrices. $\mathcal{W}_{\tau, \nu}$ is computed from ID: $\mathcal{Z}(\tau, \bar{\nu}) \mathcal{W}_{\tau, \nu} \approx\left[\mathcal{Z}\left(\tau, \overline{\nu_{1}}\right), \mathcal{Z}\left(\tau, \overline{\nu_{2}}\right)\right]$

Once all the interpolation and transfer matrices are computed, the butterfly factorization of $\mathcal{B}$ can be written as

$$
\begin{equation*}
\mathcal{Z}(o, s) \approx \mathcal{B}^{L} \mathcal{W}^{L} \mathcal{W}^{L-1} \ldots \mathcal{W}^{1} \mathcal{V}^{0} \tag{9}
\end{equation*}
$$

Here, the outer factor $\mathcal{V}^{0}=\operatorname{diag}\left(\mathcal{V}_{o, \nu_{1}}, \ldots, \mathcal{V}_{o, \nu_{2} L}\right)$ consists interpolation matrices at the leafs of $\mathfrak{T}_{s}$, and the blockdiagonal inner factors $\mathcal{W}^{l}, l=1, \ldots, L$ have blocks $\mathcal{W}_{\tau}$ for all nodes $\tau$ at level $l-1$ of $\mathfrak{T}_{o}$

$$
\left.\mathcal{W}_{\tau}=\left[\begin{array}{l}
\operatorname{diag}\left(\mathcal{W}_{\tau_{1}, \nu_{1}}, \ldots, \mathcal{W}_{\tau_{1}, \nu_{2} L-l}\right.  \tag{10}\\
\operatorname{diag}\left(\mathcal{W}_{\tau_{2}, \nu_{1}}, \ldots, \mathcal{W}_{\tau_{2}, \nu_{2} L-l}\right.
\end{array}\right)\right]
$$

Here, $\nu_{1}, \nu_{2}, \ldots, \nu_{2 L-l}$ are the nodes at level $L-l$ of $\mathfrak{T}_{s}$ and $\tau_{1}, \tau_{2}$ are children of $\tau$. Lastly, the block-diagonal outer factor $\mathcal{B}^{L}=\operatorname{diag}\left(\mathcal{Z}\left(\tau_{1}, \bar{s}\right), \ldots, \mathcal{Z}\left(\tau_{2^{L}}, \bar{s}\right)\right)$ for all leafs $\tau_{1}, \tau_{2}, \ldots, \tau_{2} L$ of $\mathfrak{T}_{o}$. Note that there exist several equivalent forms to Eq. (9) [38]-[40], [55]. Upon factorizing subblocks in $\mathcal{Z}$ in the form of Eq. (9), we obtain a compressed system matrix $\mathcal{Z}_{\chi_{c o n}}$. The storage and application costs of a matrixvector product using $\mathcal{Z}_{\chi_{c o n}}$ scale as $O(n \log n)$. As a result, the overall HOD-BF construction requires $O\left(N \log ^{2} N\right)$ memory and CPU resources (see Section III-C for more details). The HOD-BF-compressed system matrix can then be used for fast matrix-vector multiplication during the iterative solution of the VIE.


Fig. 1. Example of a $L_{H}=3$-level HOD-BF-compressed matrix. At the leaf level, the diagonal blocks $D_{\tau}$ are stored as dense blocks; at levels $l>$ $L_{H}$, the off-diagonal blocks are compressed as $L=L_{H}-l$-level butterfly representations. The HOD-BF matrix is distributed over 8 MPI processes each denoted by one color. For each $\tau, D_{\tau}$ and $\mathcal{B}_{\tau}$ are assigned to the same set of processes. $\mathcal{B}_{\tau}$ is distributed over multiple processes using parallel layouts of [55].

## B. Inversion of HOD-BF-compressed system matrix

Once constructed, the inverse of the HOD-BF-compressed system matrix can be computed approximately and used as a preconditioner during the iterative solution of Eq. (4). The inversion algorithm has been previously described in [45], [50] and is briefly summarized as HODBF_invert in Algorithm 1.

For each non-leaf $\tau, \mathcal{D}_{\tau}=\left[\mathcal{D}_{\tau_{1}}, \mathcal{B}_{\tau_{1}} ; \mathcal{B}_{\tau_{2}}, \mathcal{D}_{\tau_{2}}\right] . \mathcal{D}_{\tau}^{-1}$ is computed by first recursively computing $\mathcal{D}_{\tau_{1}}^{-1}$ and $\mathcal{D}_{\tau_{2}}^{-1}$. Next, the butterfly block is updated as $\mathcal{B}_{\tau_{i}} \leftarrow \mathcal{D}_{\tau_{i}}^{-1} \mathcal{B}_{\tau_{i}}$ with both $\mathcal{D}_{\tau_{i}}^{-1}$ and $\mathcal{B}_{\tau_{i}}$ already compressed (see line 7). Finally the updated matrix $\left[\mathcal{I}, \mathcal{B}_{\tau_{1}} ; \mathcal{B}_{\tau_{2}}, \mathcal{I}\right]$ is inverted using the butterfly extension of the Sherman-Morrison-Woodbury formula [58], named BF_SMW in Algorithm 2 (see line 8).

The operations at line 7 of Algorithm 1 and lines 3, 5 of Algorithm 2 require construction of a new butterfly representation out of combinations of existing butterfly representations. This type of operations can be accelerated by rapid multiplications of the operator with random vectors and reconstructing the butterfly from the results with tolerance $\chi_{\text {fact }}$. This algorithm is named BF_random_matvec and requires $O\left(n^{3 / 2} \log n\right)$ CPU operations [55], and consequently the computational cost for $\mathcal{Z}^{-1}$ scales as $O\left(N^{3 / 2} \log N\right)$.

```
Algorithm 1 HODBF_invert(\mathcal{A}): Inversion of a HOD-BF
matrix.
    Input: \mathcal{A in HOD-BF form}
    Output: }\mp@subsup{\mathcal{A}}{}{-1}\mathrm{ in HOD-BF form
    Let }\mp@subsup{\mathcal{D}}{\tau}{}=\mathcal{A}\mathrm{ with }\tau\mathrm{ denoting the root node.
    if }\mp@subsup{\mathcal{D}}{\tau}{}\mathrm{ dense then
        Directly compute }\mp@subsup{\mathcal{D}}{\tau}{-1
    else
        \mathcal{D}
        \mp@subsup{D}{\mp@subsup{\tau}{i}{}}{-1}}\leftarrow\mathrm{ HODBF_invert( }\mp@subsup{\mathcal{D}}{\mp@subsup{\tau}{i}{}}{}),i=1,
        \mathcal{B}}\mp@subsup{\mp@subsup{\tau}{i}{}}{}{\leftarrow
        \mp@subsup{\mathcal{D}}{\tau}{-1}}\leftarrow\mp@subsup{\textrm{BF}}{-}{}\operatorname{SMW}([\begin{array}{cc}{\mathcal{I}}&{\mp@subsup{\mathcal{B}}{\mp@subsup{\tau}{1}{}}{}}\\{\mp@subsup{\mathcal{B}}{\mp@subsup{\tau}{2}{}}{}}&{\mathcal{I}}\end{array}])[\begin{array}{cc}{\mp@subsup{\mathcal{D}}{\mp@subsup{\tau}{1}{}}{-1}}&{}\\{}&{\mp@subsup{\mathcal{D}}{\mp@subsup{\tau}{2}{}}{-1}}\end{array}
    end if
```

```
Algorithm 2 BF_SMW \((\mathcal{A})\) : SMW inversion of a butterfly
matrix.
    Input: \(\mathcal{A}-\mathcal{I}\) is a butterfly of \(L\) levels
    Output: \(\mathcal{A}^{-1}-\mathcal{I}\) is a butterfly of \(L\) levels
    Split \(\mathcal{A}\) into four children butterflies of \(L-2\) levels: \(\mathcal{A}=\)
    \(\left[\mathcal{A}_{11}, \mathcal{A}_{12} ; \mathcal{A}_{21}, \mathcal{A}_{22}\right]\) using \(\mathfrak{T}_{H}\)
    \(\mathcal{A}_{22}^{-1} \leftarrow\) BF_SMW \(\left(\mathcal{A}_{22}\right)\)
    \(\mathcal{A}_{11} \leftarrow\) BF_random_matvec \(\left(\mathcal{A}_{11}-\mathcal{A}_{12} \mathcal{A}_{22}^{-1} \mathcal{A}_{21}-\mathcal{I}\right)\)
    \(\mathcal{A}_{11}^{-1} \leftarrow\) BF_SMW \(\left(\mathcal{A}_{11}\right)\)
    \(\mathcal{A}^{-1}-\mathcal{I} \leftarrow\) BF_random_matvec
    \(\left(\left[\begin{array}{cc}\mathcal{I} & \leftarrow F_{-} \\ -\mathcal{A}_{22}^{-1} \mathcal{A}_{21} & \mathcal{I}\end{array}\right]\left[\begin{array}{cc}\mathcal{A}_{11}^{-1} & \\ & \mathcal{A}_{22}^{-1}\end{array}\right]\left[\begin{array}{cc}\mathcal{I} & -\mathcal{A}_{12} \mathcal{A}_{22}^{-1} \\ & \mathcal{I}\end{array}\right]-\mathcal{I}\right)\)
```


## C. Rank scaling and complexity estimate

We first provide a simple analysis of the butterfly rank $r$ of the off-diagonal blocks $\mathcal{B}_{\tau}$ in HOD-BF, and then summarize the complexity of the proposed HOD-BF-accelerated solver with preconditioner.

The asymptotic scaling of the butterfly ranks has been studied for various schemes, including the strong-admissibilitybased $\mathcal{H}$ matrix frameworks such as [37], [47], [48], $r=O(1)$ and weak-admissibility-based frameworks, e.g., HOD-BF. It was shown that $r=O(\log n)$ for 2-dimensional SIE [45], [46], and $r=O\left(n^{1 / 4}\right)$ for 3-dimensional SIE [55]. In what follows, we show that when applied to blocks in the 3-dimensional VIE system matrix, $r=O\left(n^{1 / 3}\right)$. Moreover, despite of the nonconstant butterfly ranks, the off-diagonal block can still be compressed with $O(n \log n)$ memory and CPU complexities using the butterfly algorithm.
To begin with, Fig. 2 shows an example of scatterer pair $(o, s)$ corresponding to one $m \times n$ block $\mathcal{Z}(o, s)$ with $L=6$, the subscatterers at level $L / 2=3$ of $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$ are shown in Fig. 2(a), and the subblocks corresponding to these subscatterer pairs are shown in Fig. 2(b). Apparently, there are $2^{L / 2}=8$ subscatterers at level $L / 2$ of both $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$, and a total of $2^{L}=64$ subblocks $\mathcal{Z}(\tau, \nu)$ for nodes $\tau, \nu=1, \ldots, 8$ at level $L / 2$. Each subscatterer contains $O\left(n^{1 / 6}\right) \times O\left(n^{1 / 6}\right) \times O\left(n^{1 / 6}\right)=O\left(n^{1 / 2}\right)$ number of unknowns. Among the $2^{L}$ subblocks, the majority $\left(O\left(2^{L}\right)\right.$ of them) representing interactions between well-separated subscatterer pairs have rank $r_{\tau, \nu}$ as $O(1)$ [36], [46], [59], [60]. There are only $O\left(2^{L / 3}\right) \approx 4$ subblocks (highlighted in red) representing interactions between face-sharing subscatterer pairs. Note that here the big O notation is needed as in practise there can be pairs partially sharing one face (i.e., non-confirming partitioning in $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$ ). The ranks of these subblocks are determined by the number of unknowns residing on the common face, leading to $r_{\tau, \nu}=O\left(n^{1 / 6}\right) \times O\left(n^{1 / 6}\right)=$ $O\left(n^{1 / 3}\right)$. Here, $O\left(n^{1 / 6}\right)$ represents the number of unknowns in one of three dimensions of a subscatterer. In addition, there can be $O\left(2^{L / 3}\right)$ subblocks representing interactions between edge-sharing or vertex-sharing subscatterer pairs whose ranks scale as $O\left(n^{1 / 6}\right)$ or $O(\log n)$. These edge-sharing or vertexsharing pairs can be safely ignored compared to the facesharing pairs. As a result, the transfer matrices $\mathcal{W}_{\tau, \nu}$ in $\mathcal{W}^{L / 2}$ require only $O\left(2^{L}\right) \times(O(1))^{2}+O\left(2^{L / 3}\right) \times\left(O\left(n^{1 / 3}\right)\right)^{2}=O(n)$
storage units. Similarly, it can be shown that any factor $\mathcal{B}^{L}, \mathcal{W}^{l}$, and $\mathcal{V}^{0}$ requires $O(n)$ memory and hence the total memory for one butterfly is $O(n \log n)$. For the same reason, the butterfly construction of $\mathcal{Z}(o, s)$ requires $O(n \log n) \mathrm{CPU}$ operations. BE CAREFUL: the entry evaluation is $O\left(r^{2}\right)$, the id is $O\left(r^{3}\right)$, but it seems entry evaluation has very large prefactors Moreover, the randomized butterfly construction BF_random_matvec used in the inversion algorithm also requires $O\left(n^{\overline{3}} / 2 \log n\right)$ CPU operations despite of the nonconstant butterfly rank [55]. Following the analysis in [45], the computational costs of the proposed HOD-BF-accelerated solver and preconditioner for VIE scale as $O\left(N \log ^{2} N\right)$ and $O\left(N^{3 / 2} \log N\right)$, respectively.


Fig. 2. (a) Subscatterers (labeled from 1 to 8 ) at level $L / 2$ of both $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$ with $L=6$. (b) Subblocks at level $L / 2$ of both $\mathfrak{T}_{o}$ and $\mathfrak{T}_{s}$. The subblocks with rank $O\left(n^{1 / 3}\right)$ are highlighted in red.

## D. Parallelization

The proposed distributed-memory parallelization scheme assigns processors according to the binary tree $\mathfrak{T}_{H}$. Let $\tau$ denote the root of $\mathfrak{T}_{H}$. Assuming a total of $P$ processors, the proposed scheme assigns all $P$ processors to $\tau$ and approximately $P / 2$ processors to each of $\tau_{1}$ and $\tau_{2}$. Recall that $\mathcal{D}_{\tau}$ is partitioned into $\left[\mathcal{D}_{\tau_{1}}, \mathcal{B}_{\tau_{1}} ; \mathcal{B}_{\tau_{2}}, \mathcal{D}_{\tau_{2}}\right]$. The first $P / 2$ processors handle $\mathcal{D}_{\tau_{1}}, \mathcal{B}_{\tau_{1}}$, and the second $P / 2$ processors handle $\mathcal{B}_{\tau_{2}}, \mathcal{D}_{\tau_{2}}$. The processor subdivision continues until the subtree rooted at one node of $\mathfrak{T}_{H}$ is entirely handled by one processor. Let $P_{\tau}$ denote the number of processors in charge of $\mathcal{D}_{\tau}$ and $\mathcal{B}_{\tau}$. The butterfly represented off-diagonal blocks $\mathcal{B}_{\tau_{1}}, \mathcal{B}_{\tau_{2}}$ are distributed using the partitioning scheme detailed in [55]. See Fig. 1 for an example of the parallel layout with 8 processors. According to this layout, Algorithms 1 and 2 are executed in parallel:

In Algorithm 1, the update operation (line 7) are handled by $P_{\tau_{i}}$ processors. As $\mathcal{D}_{\tau_{i}}^{-1}$ and $\mathcal{B}_{\tau_{i}}$ are handled by the same set of processors, no data redistribution is needed. Since there is no data dependency between nodes at each level, Algorithm 1 is highly parallelizable. On the other hand, the BF_SMW operation (line 8) is handled by $P_{\tau}$ processors. Due to the sequential nature of BF_SMW, i.e., lines 2-5 of Algorithm 2 are executed sequentially, the parallelization scheme works as follows: assuming that BF_SMW is executed on $P$ processors, a data redistribution is performed at the splitting step (line 1) where each of $\mathcal{A}_{11}, \mathcal{A}_{12}, \mathcal{A}_{21}, \mathcal{A}_{22}$ is still distributed over $P$
processors following the layout of [55]. The splitting operation proceeds with $L / 2$ levels until the children blocks become low-rank products. Note that during the splitting, the number of nonzero blocks in the children butterflies decreases and some of the $P$ processors become idle towards the leaf level of the splitting operation. To alleviate such load imbalance, each nonzero block in a butterfly can be distributed over multiple processors. Following the splitting step, no more redistribution of butterflies is needed at lines 2-5. In both Algorithm 1 and 2, the essential building block BF_random_matvec is parallelized following [55]. Note that for line 5 of Algorithm 2, the matrixvector multiplication results are not conformal to the layout of $\mathcal{A}^{-1}$, hence a data redistribution of the vectors is also required.

Overall, this scheme allows good load balance and reduced collective communication during the overall HOD-BF construction, inversion and application.

## IV. Numerical Results

This section presents several numerical examples that demonstrate the accuracy and efficiency of the proposed butterfly-accelerated VIE solver when applied to the EM analysis of heterogeneous scatterers. Unless stated otherwise below, the scatterers are illuminated by an $\hat{x}$ polarized planewave travelling along $-\hat{z}$ direction. All simulations are carried out on the Cori supercomputer of Haswell nodes; each node has two 16-core Intel Xeon E5-2698v3 processors and 128 GB of 2133 MHz DDR4 memory. Unless otherwise stated, each simulation is carried out on 16 nodes.

## A. Validation

1) Positive permittivity: First, a five-layered sphere with layer thickness of 0.06 m is analyzed. The permittivity of each layer, from outer to inner, is $2 \varepsilon_{0}, 3 \varepsilon_{0}, 4 \varepsilon_{0}, 5 \varepsilon_{0}$ and $6 \varepsilon_{0}$ [Fig. 3(a)]. The sphere is discretised by a tetrahedral mesh with $N=407,842$, and the radar cross section (RCS) of the sphere is computed at $f=750 \mathrm{MHz}$ using the proposed VIE solver with compression tolerance $\chi_{\text {con }}=10^{-4}$, factorization tolerance $\chi_{\text {fact }}=10^{-1}$, and TFQMR stopping criteria $\chi_{\text {sol }}=10^{-3}$. The computed RCS is compared with the one obtained via (exact) Mie series solution [Fig. 3(b)]. Let $x_{i}$ and $\hat{x}_{i}, i=1, \ldots, N_{r c s}$ denote the $N_{r c s}$ RCS samples computed by the proposed solver and Mie series solution, respectively. The relative root-mean-square error (RMSE) is defined as $\sqrt{\sum_{i}\left(x_{i}-\hat{x}_{i}\right)^{2} / N_{r c s}} / \max _{i} \hat{x}_{i}$, where $x_{i}$ are in their original values rather than in dBsm . The relative RMSE between two solutions is 0.024 . The good agreement between results shows that the proposed VIE solver with the chosen parameters achieve good accuracy. It should be noted that the proposed solver requires 2 and 78 TFQMR iterations with and without preconditioner, respectively. The details of the simulation performed by the proposed solver are provided in Table I.

Next, a three-layered sphere with a hollow spherical core (i.e., two shells) is analyzed. The sphere has a radius of 2.4 m and each shell has thickness of 0.03 m . The dielectric permittivity of each shell, from inner to outer, is $4 \varepsilon_{0}$ and $2 \varepsilon_{0}$, respectively [Fig. 4]. The tetrahedral mesh of two shells


Fig. 3. (a) The structure considered for the analysis: a five-layered sphere with $\varepsilon_{1}=2 \varepsilon_{0}, \varepsilon_{2}=3 \varepsilon_{0}, \varepsilon_{3}=4 \varepsilon_{0}, \varepsilon_{4}=5 \varepsilon_{0}$, and $\varepsilon_{5}=6 \varepsilon_{0}$. (b) The RCSs computed by the proposed HOD-BF-accelerated VIE solver and Mie series solution at $f=750 \mathrm{MHz}$.
consists of $N=5,530,950$ faces. The RCS is computed at $f=600 \mathrm{MHz}$ using the proposed VIE solver with $\chi_{\text {con }}=10^{-4}$, $\chi_{\text {fact }}=10^{-1}$, and $\chi_{\text {sol }}=10^{-3}$. The computed RCS is compared with the one obtained via the Mie series solution [Fig. 4(b)]. The relative RMSE between two solutions is 0.0034 . Once again, the results show very good agreement. The proposed VIE solver with and without preconditioner requires 7 and 643 TFQMR iterations, respectively. More details on the simulation are provided in Table I.


Fig. 4. (a) The structure considered for the analysis: a two-layered shell with $\varepsilon_{1}=2 \varepsilon_{0}$, and $\varepsilon_{2}=4 \varepsilon_{0}$. (b) The RCSs computed with the proposed HOD-BF-accelerated VIE solver and Mie series solution at $f=600 \mathrm{MHz}$.

TABLE I
TECHNICAL DATA FOR THE NUMERICAL EXAMPLES: LAYERED SPHERE, SHELL, AND SPHERE WITH NEGATIVE PERMITTIVITY.

| Example | Layered | Shell | Negative Sphere |
| :---: | :---: | :---: | :---: |
| Max. dimension | $1.5 \lambda_{0}$ | $9.6 \lambda_{0}$ | $1.6 \lambda_{0}$ |
| $N$ | 407,842 | $5,530,950$ | 896,001 |
| Max. rank | 1088 | 1331 | 1198 |
| Memory for $\mathcal{Z}$ | 57 GB | 324 GB | 96 GB |
| Memory for $\mathcal{Z}^{-1}$ | 28 GB | 321 GB | 306 GB |
| Construction time | 7.4 min | 1.5 h | 1.9 h |
| Inversion time | 26 min | 6.2 h | 6.5 h |
| Solve time w/ precond. | 2.3 s | 48.3 s | 21.4 s |
| Iteration \# w/ precond. | 2 | 7 | 6 |
| Solve time w/o precond. | 42.8 s | 32 min | 46 min |
| Iteration \# w/o precond. | 78 | 643 | 3447 |

2) Negative permittivity: In general, the VIE formulation results in poorly conditioned systems when applied to the
scattering problems involving negative permittivity. Iterative solution of such systems often do not converge with simple or no preconditioners. However, the use of HOD-BF with increased accuracy in factorization and solution provides stable and accurate results, even for the ill-conditioned systems. To demonstrate the stability and accuracy of the proposed simulator for such systems, a sphere of radius 0.3 m with permittivity $\varepsilon(\mathbf{r})=(-4-0.2 j) \varepsilon_{0}$ is analyzed. The sphere is discretized by a tetrahedral mesh consisting of $N=896,001$ faces. The RCS is computed at $f=800 \mathrm{MHz}$ using the proposed VIE solver with $\chi_{\text {con }}=10^{-4}$, $\chi_{\text {fact }}=10^{-3}$, and $\chi_{\text {sol }}=10^{-5}$. The computed RCS is compared with the one obtained by the analytical Mie series solution [Fig. 5(b)]; The relative RMSE between two solutions is 0.0027 . It is a well-known fact that the discretized VIE system becomes ill-conditioned for the EM analysis of the scatterers with negative permittivity and the iterative solution of the VIE system oftentimes cannot be obtained [21], [24], [61]. Here the proposed VIE solver with preconditioner obtains the solution after 6 TFQMR iterations. Note that the choice of $\chi_{\text {fact }}=10^{-3}$ represents a trade-off between inversion time and solve time. This clearly shows that the proposed solver is less sensitive to the ill-conditioning due to negative permittivity and it is robust for the board permittivity EM analysis. This example was run on 16 nodes and the details of the simulation are provided in Table I.


Fig. 5. (a) The structure considered for the analysis: a sphere with negative permittivity, $\varepsilon(\mathbf{r})=(-4-0.2 j) \varepsilon_{0}$. (b) The RCSs computed via the proposed HOD-BF-accelerated VIE solver and Mie series solution at $f=800$ MHz.

## B. Computational Complexity

In this subsection, several examples were considered to verify the predicted CPU and memory scaling of the proposed HOD-BF-accelerated VIE solver. In all examples, the scatterers are discretized by the tetrahedal mesh with elements comparable to $\lambda_{0} / 10$. The performance of the proposed HOD-BF-accelerated VIE solver is compared with that of an $\mathcal{H}$ matrix-accelerated VIE solver with strong admissibility, and an HOD-LR-accelerated VIE solver. For the $\mathcal{H}$ matrixaccelerated solver, all low-rank matrix blocks corresponding to $d_{a, b}>\alpha \max \left(r_{a}, r_{b}\right)$ are compressed, where $r_{a}$ and $r_{b}$ are the radii of the spheres enclosing subscatterers $a$ and $b, d_{a, b}$ is the distance between the centers of subscatterers, and $\alpha=2$. We used a cobblestone distance sorting-based partitioning [62] in the $\mathcal{H}$ matrix, HOD-LR, and HOD-BF
accelerated solvers. For the low-rank compression algorithms, we used a blocked variant of adaptive cross approximation algorithm [63] for better stability and parallel performance. The $\mathcal{H}$ matrix solver and HOD-LR solvers are available in the open-source software ButterflyPACK. In the following tests, $\chi_{\text {con }}=10^{-3}, \chi_{\text {fact }}=10^{-1}$, and $\chi_{\text {sol }}=10^{-3}$.


Fig. 6. (a) The CPU and (b) memory scaling of the HOD-BF-accelerated solver, $\mathcal{H}$ matrix-accelerated solver, and HOD-LR-accelerated solver when applied to the EM analysis of a sphere with permittivity $\varepsilon(\mathbf{r})=$ $(4-0.0001 j) \varepsilon_{0}$.


Fig. 7. (a) CPU and (b) memory scaling of the HOD-BF-accelerated solver and $\mathcal{H}$ matrix-accelerated solver when applied to the EM analysis of a NASA almond with permittivity $\varepsilon(\mathbf{r})=(4-0.0001 j) \varepsilon_{0}$

1) Positive permittivity: The computational complexity of the proposed scheme is studied as a function of electrical size by varying the frequency and fixing object size, or, by keeping the frequency fixed and varying the object size. In the first example, EM analysis of an homogeneous sphere


Fig. 8. (a) The CPU and (b) memory scaling of the HOD-BF-accelerated solver and $\mathcal{H}$ matrix-accelerated solver when applied to the EM analysis of a two-layered shell with inner and outer shell permittivities of $4 \varepsilon_{0}$ and $2 \varepsilon_{0}$

TABLE II
TIME (IN SECONDS) AND ITERATION COUNT FOR THE SOLVE PHASE OF THE PROPOSED HOD-BF-ACCELERATED VIE SOLVER WITH ('W/') AND Without ('w/o') Preconditioner. Note that each TFQMr ITERATION REQUIRES 6 MVPs.

| $N$ | 225,746 | 538,782 | 896,001 | $1,757,024$ |
| :---: | :---: | :---: | :---: | :---: |
| Solve time w/ | 1.3 | 3.3 | 6.77 | 17 |
| Iteration \# w/ | 3 | 3 | 4 | 5 |
| Time per MVP w/ | 0.07 | 0.185 | 0.28 | 0.56 |
| Solve time w/o | 48.9 | 310.1 | 509.2 | 1940 |
| Iteration \# w/o | 279 | 712 | 786 | 1535 |
| Time per MVP w/o | 0.03 | 0.07 | 0.11 | 0.21 |

TABLE III
TECHNICAL DATA FOR THE EXAMPLES: SPHERE, ALMOND, HUMAN HEAD

| Example | Sphere | Almond | Head |
| :---: | :---: | :---: | :---: |
| Max. dimension | $3.4 \lambda_{0}$ | $10 \lambda_{0}$ | $0.662 \lambda_{0}$ |
| $N$ | $1,757,024$ | $2,972,024$ | $1,759,208$ |
| Max. rank | 1496 | 2006 | 1981 |
| Memory for $\mathcal{Z}$ | 148 GB | 228 GB | 314 GB |
| Memory for $\mathcal{Z}^{-1}$ | 170 GB | 241 GB | 353 GB |
| Construction time | 22 min | 1.5 h | 3 h |
| Inversion time | 4.2 h | 7.4 h | 7.3 h |
| Solve time w/ precond. | 17 s | 24 s | 5.4 min |
| Iteration \# w/ precond. | 5 | 4 | 90 |
| Solve time w/o precond. | 32 min | 35 min | 1.8 h |
| Iteration \# w/o precond. | 1535 | 962 | 3698 |

with radius 0.3 m and permittivity $\varepsilon(\mathbf{r})=(4-0.0001 j) \varepsilon_{0}$ is considered for frequencies $700 \mathrm{MHz}, 850 \mathrm{MHz}, 1.2 \mathrm{GHz}, 1.3$ $\mathrm{GHz}, 1.6 \mathrm{GHz}, 2.0 \mathrm{GHz}, 2.5 \mathrm{GHz}$, and 2.8 GHz . The analysis at 2.8 GHz requires a tetrahedral mesh with $N=12,455,135$. Comparison of the complexities of the $\mathcal{H}$ matrix-accelerated solver and the proposed HOD-BF-accelerated solver in Fig. 6 reveals that the CPU time for HOD-BF construction and inversion scale as $O\left(N \log ^{2} N\right)$ and $O\left(N^{1.5} \log N\right)$, respectively and the memory requirement scales as $O\left(N \log ^{2} N\right)$. These
scaling results match with the predicted ones in Section III-C. The maximum butterfly rank ranges from 745 to 2800 , which scales as $O\left(N^{1 / 3}\right)$. In contrast, the inversion and memory cost of $\mathcal{H}$ matrix-accelerated solver scale roughly $O\left(N^{2}\right)$ and $O\left(N \log ^{2} N\right)$, respectively. In addition, its construction cost scales with $O\left(N^{1.5}\right)$, although the scaling plot was not provided in Fig. 6 to avoid overcrowding. In addition, the proposed HOD-BF-accelerated solver requires four times less memory compared to $\mathcal{H}$ matrix-accelerated solver. Moreover, the HOD-LR VIE solver scales as $O\left(N^{5 / 3}\right)$ for memory and $O\left(N^{7 / 3}\right)$ for CPU. Due to its prohibitively high CPU and memory requirement for 3D VIE, we do not consider HODLR solvers for the other experiments.

The solution obtained via HOD-BF-accelerated solver without preconditioner, which only requires performing HOD-BF construction, will not converge to $\chi_{\text {sol }}=10^{-3}$ within 3000 iterations when the electrical size of the object is large. For example, iterative solution via such solver requires 167 iterations for $N=13,3207,1535$ iterations for $N=1,757,024$, and fails to converge for larger problems. In contrast, the HOD-BF-accelerated solver with preconditioner requires at most 5 iterations for the analysis at all frequencies. The data for the solve phase of HOD-BF-accelerated VIE solver with and without preconditioner is provided in Table II. As $N$ increases, the discretized VIE system becomes increasingly ill-conditioned, yet the approximate inverse preconditioner remains very effective and allows retaining the number TFQMR iterations a few. The time for each matrix-vector product (MVP) with the preconditioner is about twice of that without the preconditioner. The technical data for $N=1,757,024$ is provided in Table III.

Next, a NASA almond with size $0.25 \times 0.1 \times 0.04 \mathrm{~m}$ and permittivity $\varepsilon(\mathbf{r})=(4-0.0001 j) \varepsilon_{0}$ is considered to study the computational complexity for frequencies $4.4,5.4,6.7,8$, $10,12,15$, and 20 GHz . The analysis at 20 GHz requires a tetrahedral mesh with $N=12,112,059$. Fig. 7 shows that the CPU and memory requirements of the HOD-BF-accelerated solver for the construction and inversion scale as those predicted in Section III-C. In contrast, the CPU scaling of the $\mathcal{H}$ matrix-accelerated solver for the construction and inversion is at least $O\left(N^{1.5}\right)$. Again, the iterative solution via HOD-BFaccelerated solver without preconditioner does not converge for the meshes with more than $N=2,972,024$ elements. However, the HOD-BF-accelerated solver with preconditioner requires maximum 4 TFQMR iterations for the analysis at all frequencies. More details on the analysis with the mesh comprising $N=2,972,024$ elements are provided in Table III.

Furthermore, a three-layered sphere with a hollow spherical core (i.e., two shells) illuminated by a plane wave at 600 MHz is considered for the complexity analysis. The permittivities of inner and outer shells with thickness of 0.03 m are $4 \varepsilon_{0}$ and $2 \varepsilon_{0}$, respectively. The radius of the sphere is increased from 0.3 m to 4.8 m ; the sphere with the largest radius requires a mesh with $N=22,491,763$. Fig. 8 shows that the CPU and memory requirements of the HOD-BF-accelerated solver for the construction and inversion scale as those predicted in Section III-C. Note that the memory requirement and
construction time behave slightly better than the predicted $O\left(N \log ^{2} N\right)$ scaling. For this example, the scalings for the $\mathcal{H}$ matrix-accelerated solver are similar to those of the proposed solver, but with much larger leading constants. More details on the analysis with the mesh comprising $N=5,530,950$ elements are provided in Table I.
2) Negative Permittivity: In the next example, a sphere with permittivity $\varepsilon(\mathbf{r})=(-4-2 j) \varepsilon_{0}$ is analyzed for frequencies $700 \mathrm{MHz}, 900 \mathrm{MHz}, 1.2 \mathrm{GHz}, 1.4 \mathrm{GHz}$, and 1.7 GHz . The analysis at 1.7 GHz requires a mesh with $N=1,757,024$.

Fig. 9 shows that the construction and inversion costs of the proposed HOD-BF-accelerated solver scale as $O\left(N \log ^{2} N\right)$ and $O\left(N^{1.5} \log N\right)$, respectively; its memory requirement scales as $O\left(N \log ^{2} N\right)$; the maximum butterfly rank scales as $O\left(N^{1 / 3}\right)$. All the scaling results match the predicted ones in Section III-C. Note that the solve time is also plotted (in blue) in Fig. 9(a), which is negligible compared to the construction and inversion times, since the TFQMR iteration count is maximum 12 for the analyses at all frequencies.

From the analysis in this subsection, we can conclude that the proposed HOD-BF-accelerated solver requires much less CPU time and memory compared to $\mathcal{H}$ matrix-accelerated solver when the electrical size of the scatterer is large. Indeed, the complexities of $\mathcal{H}$ matrix-accelerated solver strongly depend on the geometry of the structure and can scale as bad as $O\left(N^{2}\right)$. Furthermore, it is clear that the proposed simulator can provide efficient and accurate EM analysis even for the problems necessitating the solution of ill-conditioned VIE systems.


Fig. 9. (a) The CPU and (b) memory scaling of the HOD-BF-accelerated solver and $\mathcal{H}$ matrix-accelerated solver when applied to the EM analysis of a sphere with permittivity $\varepsilon(\mathbf{r})=(-4-2 j) \varepsilon_{0}$

## C. Biomedical Application

The proposed HOD-BF-accelerated VIE solver is applied to the characterization of EM fields inside a human head induced by a cellphone operated at 900 MHz . To this end, a head model
is discretized using tetrahedrons with an average volume of 1 $\mathrm{mm}^{3}$; the resulting mesh has $N=1,759,208$ faces. The head model is excited by a $z$-directed dipole positioned near to the ear. The relative permittivities of the tissues are plotted in Fig. 10; those range from $12.50-j 2.86$ to $68.60-j 48.134$. The electric fields induced inside the human head is computed using the proposed HOD-BF-accelerated solver [Fig. 11].

The HOD-BF-accelerated solver with $\chi_{c o n}=10^{-3}$, $\chi_{\text {fact }}=10^{-1}$ and $\chi_{\text {sol }}=10^{-5}$ requires 45 and 2568 TFQMR iterations with and without the preconditioner, respectively. This example was run on 32 nodes and the details of the simulation are provided in Table III.


Fig. 10. The profile of the (a) real and (b) imaginary parts of the relative permittivities of tissues in the head model at 900 MHz .


Fig. 11. (a) Right view and (b) left view of the magnitude of the electric field (in $\log$ scale) inside the human head excited by a dipole with $1 \mathrm{~mA}-\mathrm{m}$ strength at 900 MHz computed by the proposed HOD-BF-accelerated solver.

## V. Conclusion

In this paper, a butterfly-accelerated VIE solver for the EM analysis of electrically-large scatterers comprising of broad permittivity values was proposed. The solver constructs the HOD-BF compressed blocks in the VIE system and accelerates the matrix-vector multiplications using these blocks. Furthermore, it leverages a preconditioner formed by the approximate inverse of the system matrix to ensure the fast convergence of the iterative solution. The complexity analysis and numerical experiments confirmed $O\left(N \log ^{2} N\right) \mathrm{CPU}$ and memory scaling of the proposed solver for the construction of HOD-BF compressed blocks. Moreover, an $O\left(N^{1.5} \log N\right)$ CPU time scaling and $O\left(N \log ^{2} N\right)$ memory scaling were validated for the inversion of the system matrix to form the preconditioner. The proposed HOD-BF-accelerated VIE solver was applied to EM analyses of various canonical and realistic scatterers. It was shown that the proposed solver can achieve significant CPU and memory savings compared to the low-rank-based $\mathcal{H}$ matrix-accelerated VIE solver for the highfrequency EM analysis.

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