A Butterfly-Accelerated Volume Integral Equation Solver for Large-Scale Electromagnetic Analysis

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***Abstract*—A butterfly acceleration scheme is proposed for the fast solution of volume integral equation (VIE). The proposed scheme efficiently constructs the method of moments (MoM) matrix in the compressed format and obtains an approximate inverse of the MoM matrix, used as a highly effective preconditioner. The proposed scheme enables to efficiently solve problems involving millions of unknowns. Furthermore, it requires much less computational resources compared to $\mathcal{H}$ matrix scheme for the electromagnetic (EM) scattering analysis of electrically large structures.**

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

I. Introduction

RECENT advances in EM and optical systems require fast and accurate simulation tools to characterize EM scattering from heterogeneous structures. Among various tools developed for this purpose, VIE solvers offer several advantages over their differential equation counterparts. The VIE solvers require the solution of a dense linear system of equations (LSE), which has to be accelerated by a fast matrix-vector multiplication scheme (such as the ones based on fast multipole method and/or fast Fourier transform [1]–[5]). Oftentimes, the LSE becomes ill-conditioned when analyzing the structures with negative permittivity [6], [7], high permittivity [8]–[10], or mixed positive and negative permittivity [11]. This ill-conditioning results in slow or no convergence of the iterative solution of the LSE. To this end, fast schemes to accelerate the matrix-vector multiplications as well as the convergence of the iterative solutions are highly desirable for the broad permittivity and large-scale EM analysis of heterogeneous structures.

In this study, a hierarchical off-diagonal butterfly (HOD-BF) scheme [12] is proposed for the fast solution of LSE in VIE solvers. The scheme efficiently constructs the HOD-BF-compressed matrix blocks, used for the fast matrix-vector multiplication during the iterative solution of LSE. Moreover, the scheme obtains a cheap and approximate inverse of the MoM matrix, used as a highly effective preconditioner. Such preconditioner reduces the number of iterations to single digit even for highly ill-conditioned LSEs, arising in the analyses pertinent to the structures with negative, high, or mixed permittivity. The computational time required by the proposed scheme to obtain the HOD-BF-compressed blocks and to perform multiplication with them scales as $O(N\log^2 N)$, while that required to obtain the approximate inverse preconditioner scales as $O(N^{1.5}\log N)$. Here N is the number of Schaubert-Wilton-Glisson (SWG) functions [13] used to discretize the flux in the analyzed structure.

II. VIE Formulation

Assume that a time-harmonic EM field is incident upon a heterogeneous structure with dielectric permittivity $\varepsilon(\mathbf{r})$ and the structure resides in a background medium with permittivity ε_0. The electric flux inside the structure can be obtained by solving the LSE, which reads

$$\mathbf{ZI} = \mathbf{V}, \tag{1}$$

where

$$\begin{aligned} Z(m,n) &= \left\langle \mathbf{f}_m(\mathbf{r}), \frac{\mathbf{f}_n(\mathbf{r})}{\varepsilon(\mathbf{r})} - j2\pi f\eta\mathcal{L}\left(\kappa(\mathbf{r})\mathbf{f}_n(\mathbf{r})\right)\right\rangle_m \\ I(n) &= D_n \\ V(m) &= \left\langle \mathbf{f}_m(\mathbf{r}), \mathbf{E}^{\mathbf{inc}(\mathbf{r})}\right\rangle_m; \qquad n,m = 1,...,N. \end{aligned} \tag{2}$$

In (2), $\mathbf{f}_n(\mathbf{r})$ is the SWG basis function with the unknown expansion coefficient D_n, f is the frequency, η is intrinsic impedance, $\mathcal{L}$ is the EFIE operator [9], $\kappa(\mathbf{r}) = (\varepsilon(\mathbf{r}) - \varepsilon_0)/\varepsilon(\mathbf{r})$ is the contrast, $\mathbf{E}^{\mathrm{inc}}(\mathbf{r})$ is the incident electric field, and $< \mathbf{a}, \mathbf{b} >_m$ denotes the standard inner product of $\mathbf{a}$ with $\mathbf{b}$ on the support of m^{th} testing function. The construction of MoM matrix $\mathbf{Z}$ and its iterative solution for $\mathbf{I}$ require $O(N^2)$ computational resources; such cost can be reduced to $O(N\log^2 N)$ via the proposed HOD-BF scheme.

III. HOD-BF Acceleration and Preconditioner

The proposed HOD-BF scheme is a high-frequency extension of the hierarchically off-diagonal low-rank (HOD-LR) scheme. The HOD-LR scheme generates a hierarchical partitioning of the MoM matrix followed by compression of off-diagonal blocks representing non-overlapping interactions as low-rank products. The compressed blocks permit fast matrix-vector multiplications and inversion at low-frequency EM analysis. The HOD-BF scheme replaces the low-rank products in HOD-LR scheme with butterflies to enable high-frequency compression. The construction of the HOD-BF-compressed MoM matrix and approximate inverse preconditioner are described below:

A. Construction of HOD-BF-compressed MoM matrix

The construction begins by recursively subdividing the scatterer (i.e., structure) into subscatterers with approximately equal numbers of unknowns using a tree clustering algorithm

[14]. This procedure yields a complete binary tree $\mathcal{T}_H$ of L_H levels with root level 0 and leaf level L_H. Each node τ at level l is an index set $\tau \subset \{1,\ldots,N\}$ associated with the corresponding subscatterer. For a non-leaf node τ at level l with children τ_1 and τ_2, $\tau = \tau_1 \cup \tau_2$ and $\tau_1 \cap \tau_2 = \emptyset$. For a non-root node τ, its parent is denoted p_τ. At the leaf level, the diagonal blocks $\mathbf{D}_\tau = \mathbf{Z}(\tau,\tau)$ are directly computed as dense blocks, while off-diagonal blocks are compressed using the butterfly representation described below.

Specifically, let τ_1 and τ_2 be two siblings in $\mathcal{T}_H$ on level l. These two sibling nodes correspond to two off-diagonal blocks $\mathbf{B}_{\tau_1} = \mathbf{Z}(\tau_1,\tau_2)$ and $\mathbf{B}_{\tau_2} = \mathbf{Z}(\tau_2,\tau_1)$. As an example consider the butterfly compression of the $m\times n$ block $\mathbf{B} = \mathbf{B}_{\tau_1}$ with $o = \tau_1$ and $s = \tau_2$, then $\mathbf{B} = \mathbf{Z}(o,s)$ is compressed as a butterfly with $L = L_H - l$ levels. Let $\mathcal{T}_o$ and $\mathcal{T}_s$ denote subtrees of $\mathcal{T}_H$ with L levels, rooted at nodes o and s respectively. The butterfly compression requires the *complementary low-rank property*: for any level $0 \le l \le L$, any node τ at level l of $\mathcal{T}_o$ and any node ν at level $L-l$ of $\mathcal{T}_s$, the subblock $\mathbf{Z}(\tau,\nu)$ is numerically low-rank with rank $r_{\tau,\nu}$ bounded by a small number r called the butterfly rank. Given the complementary low-rank property, we can compress any subblock $\mathbf{Z}(\tau,\nu)$ above as a low-rank product in an interpolative form:

$$\mathbf{Z}(\tau,\nu) \approx \mathbf{Z}(\tau,\bar{\nu})\mathbf{V}_{\tau,\nu}. \tag{3}$$

where $\bar{\nu}$ represents the skeleton columns, $\mathbf{Z}(\tau,\bar{\nu})$ is the skeleton matrix, and $\mathbf{V}_{\tau,\nu}$ is the interpolation matrix. Once all the interpolation and transfer matrices are computed, the butterfly factorization of $\mathbf{B}$ can be written as

$$\mathbf{Z}(o,s) \approx \mathbf{B}^L\mathbf{W}^L\mathbf{W}^{L-1}\ldots\mathbf{W}^1\mathbf{V}^0. \tag{4}$$

Here, the outer factor $\mathbf{V}^0 = \mathrm{diag}(\mathbf{V}_{o,\nu_1},\ldots,\mathbf{V}_{o,\nu_{2^L}})$ consists interpolation matrices at the leafs of $\mathcal{T}_s$, and the block-diagonal inner factors $\mathbf{W}^l, l = 1,\ldots,L$ have blocks $\mathbf{W}_\tau$ for all nodes τ at level $l-1$ of $\mathcal{T}_o$.

B. Inversion of HOD-BF-compressed system matrix

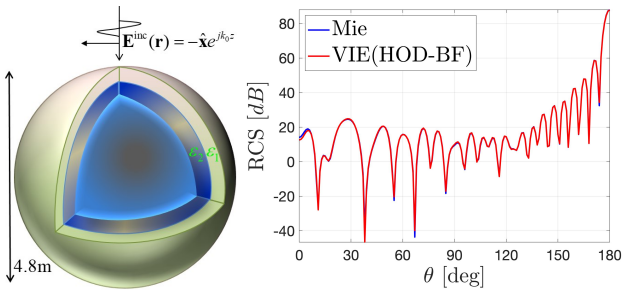
Once constructed, the inverse of the HOD-BF-compressed system matrix can be computed approximately and used as a preconditioner during the iterative solution of Eq. (1). The inversion algorithm has been previously described in [12], [15].

Let $\mathbf{D}_\tau = \mathbf{Z}(\tau,\tau)$ denote the diagonal block associated with node τ at level l of $\mathcal{T}_H$. The recursive algorithm essentially starts from level $l = L_h$ and inverts the dense $\mathbf{D}_\tau$ directly. For node τ at higher levels l, it is not hard to see that $\mathbf{D}_\tau$ is a HOD-BF matrix with $L_h - l$ levels. $\mathbf{D}_\tau$ is then partitioned into $[\mathbf{D}_{\tau_1},\mathbf{B}_{\tau_1};\mathbf{B}_{\tau_2},\mathbf{D}_{\tau_2}]$. $\mathbf{D}_{\tau_1}^{-1}$ and $\mathbf{D}_{\tau_2}^{-1}$ are first computed by recursion. Next, the butterfly block is updated as $\mathbf{B}_{\tau_i} \leftarrow \mathbf{D}_{\tau_i}^{-1}\mathbf{B}_{\tau_i}$ with both $\mathbf{D}_{\tau_i}^{-1}$ and $\mathbf{B}_{\tau_i}$ already compressed. Finally the updated matrix $[\mathbf{I},\mathbf{B}_{\tau_1};\mathbf{B}_{\tau_2},\mathbf{I}]$ is inverted using the butterfly extension of the Sherman-Morrison-Woodbury formula [16]. The algorithm also computes a butterfly approximation of $\mathbf{Z}^{-1}$ with a relative tolerance to be used as a preconditioner.

IV. Numerical Results

Two numerical examples to demonstrate the accuracy and efficiency of the proposed solver are presented here. In both examples the structures are illuminated by an $\hat{x}$ polarized plane-wave 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 and each simulation is carried out on 16 nodes.

In the first example, a two-layered spherical shell is considered. The shell has a outer radius of 2.4 m with thickness of 0.03 m for both layers and permittivity of $4\varepsilon_0$ for the inner layer and $2\varepsilon_0$ for the outer layer [Fig. 1]. The flux inside the structure is discretized by $N = 5,530,950$ SWG basis functions. The radar cross section (RCS) is computed at $f = 600$ MHz using the proposed VIE solver and compared with analytical Mie series solution [Fig. 1(b)]; both results demonstrate very good agreement. The required number of iterations with and without approximate inverse preconditioner are 7 and 643, respectively. This shows the effectiveness of the proposed preconditioner.



(a) (b)

Fig. 1. (a) Two-layered shell with $\varepsilon_1 = 2\varepsilon_0$, and $\varepsilon_2 = 4\varepsilon_0$. (b) The RCSs computed with the proposed solver and Mie series solution at $f = 600$ MHz.

In the second example, a NASA almond with size $0.25 \times 0.1 \times 0.04$ m and permittivity $\varepsilon(\mathbf{r}) = (4 - 0.0001j)\,\varepsilon_0$ is analyzed. The computational and memory requirements of the proposed scheme are studied while the frequency is changed from 4.4 GHz to 20 GHz with maximum $N = 12,112,059$. Fig. 2 shows that the construction cost of compressed MoM matrix in the HOD-BF-accelerated solver scales as $O(N\log^2 N)$. In contrast, the construction cost required in the low-rank $\mathcal{H}$ matrix-accelerated solver scales at least $O(N^{1.5})$. In addition, the computational cost of inversion to obtain preconditioner scales as $O(N^{1.5}\log N)$ for both HOD-BF and $\mathcal{H}$ matrix schemes. For the analysis with $N = 1.6$M unknowns, HOD-BF scheme requires 5.0x/3.2x less computational time and 3.2x/2.7x less memory compared to the $\mathcal{H}$ matrix scheme for the construction/inversion. The iterative solution via HOD-BF-accelerated solver without preconditioner does not converge for the analyses with more than $N = 3$M unknowns. However, the HOD-BF-accelerated solver with preconditioner requires maximum 4 iterations for the analyses at all frequencies.

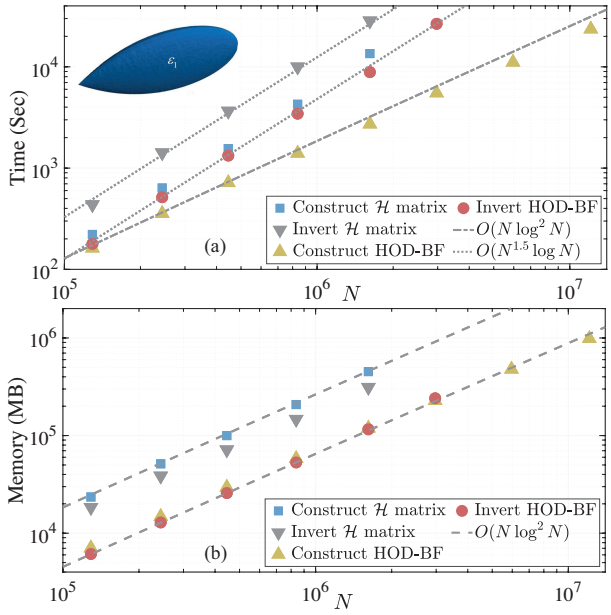


Fig. 2. (a) CPU and (b) memory scaling of the HOD-BF-accelerated solver and $\mathcal{H}$ matrix-accelerated solver when applied to the EM analysis of a NASA almond with permittivity $\varepsilon(\mathbf{r}) = (4 - 0.0001j)\,\varepsilon_0$

REFERENCES

[1] C.-C. Lu, "A fast algorithm based on volume integral equation for analysis of arbitrarily shaped dielectric radomes," *IEEE Trans. Antennas Propag.*, vol. 51, no. 3, pp. 606–612, 2003.

[2] M. F. Catedra, E. Gago, and L. Nuno, "A numerical scheme to obtain the rcs of three-dimensional bodies of resonant size using the conjugate gradient method and the fast fourier transform," *IEEE Trans. Antennas Propag.*, vol. 37, no. 5, pp. 528–537, 1989.

[3] A. C. Yucel, I. Georgakis, A. G. Polimeridis, H. Bagci, and J. White, "VoxHenry: A fast Fourier transform - accelerated 3D inductance extraction program for voxelized geometries," *IEEE Trans. Microwave Theory Tech.*, vol. 66, no. 4, pp. 1723–1735, 2018.

[4] M. Wang, C. Qian, J. K. White, and A. C. Yucel, "VoxCap: FFT-accelerated and Tucker-enhanced capacitance extraction simulator for voxelized structures," *IEEE Trans. Microw. Theory Techn.*, vol. 68, no. 12, pp. 5154–5168, 2020.

[5] A. C. Yucel, W. Sheng, C. Zhou, Y. Liu, H. Bagci, and E. Michielssen, "An fmm-fft accelerated sie simulator for analyzing em wave propagation in mine environments loaded with conductors," *IEEE Journal on Multiscale and Multiphysics Comp. Techn.*, vol. 3, pp. 3–15, 2018.

[6] A. C. Yucel, L. J. Gomez, and E. Michielssen, "Internally combined volume-surface integral equation for em analysis of inhomogeneous negative permittivity plasma scatterers," *IEEE Trans. Antennas Propag.*, vol. 66, no. 4, pp. 1903–1913, 2018.

[7] L. J. Gomez, A. C. Yucel, and E. Michielssen, "Volume-surface combined field integral equation for plasma scatterers," *IEEE Antennas Wireless Propag. Lett.*, vol. 14, pp. 1064–1067, 2015.

[8] ——, "Low-frequency stable internally combined volume-surface integral equation for high-contrast scatterers," *IEEE Antennas Wireless Propag. Lett.*, vol. 14, pp. 1423–1426, 2015.

[9] ——, "Internally combined volume-surface integral equation for a 3-d electromagnetic scattering analysis of high-contrast media," *IEEE Antennas Wireless Propag. Lett.*, vol. 16, pp. 1691–1694, 2017.

[10] ——, "The icvsie: A general purpose integral equation method for bio-electromagnetic analysis," *IEEE Trans. Biomed. Eng.*, vol. 65, no. 3, pp. 565–574, 2017.

[11] S. B. Sayed, A. C. Yucel, and L. J. Gomez, "A multi-region internally combined volume surface integral equation for em analysis of inhomogeneous negative and positive permittivity scatterers," in *2020 IEEE USNC-CNC-URSI North American Radio Science Meeting (Joint with AP-S Symposium)*, 2020, pp. 185–186.

[12] Y. Liu, H. Guo, and E. Michielssen, "An HSS matrix-inspired butterfly-based direct solver for analyzing scattering from two-dimensional objects," *IEEE Antennas Wirel. Propag. Lett.*, vol. 16, pp. 1179–1183, 2017.

[13] D. Schaubert, D. Wilton, and A. Glisson, "A tetrahedral modeling method for electromagnetic scattering by arbitrarily shaped inhomogeneous dielectric bodies," *IEEE Trans. Antennas Propag.*, vol. 32, no. 1, pp. 77–85, 1984.

[14] H. Guo, J. Hu, and E. Michielssen, "On MLMDA/butterfly compressibility of inverse integral operators," *IEEE Antennas Wirel. Propag. Lett.*, vol. 12, pp. 31–34, 2013.

[15] Y. Liu, P. Ghysels, L. Claus, and X. S. Li, "Sparse approximate multifrontal factorization with butterfly compression for high frequency wave equations," *arXiv e-prints*, p. arXiv:2007.00202, Jun. 2020.

[16] W. W. Hager, "Updating the inverse of a matrix," *SIAM Review*, vol. 31, no. 2, pp. 221–239, 1989.