



A Comparative Study of Butterfly-enhanced Direct Integral and Differential Equation Solvers for High-frequency Electromagnetic Analysis Involving Inhomogeneous Dielectrics

Yang Liu⁽¹⁾

(1) The Lawrence Berkeley National Laboratory, Berkeley, CA, 94706

Abstract

We compare the performance of three butterfly-accelerated direct integral and differential equation solvers for modeling high-frequency time-harmonic electromagnetic interaction with inhomogeneous dielectrics. The three solvers are based on finite-difference frequency-domain (FDFD) method, volume integral equation (VIE), and Babich expansion-based surface integral equation (SIE), respectively. Despite of the reduced complexity with butterfly acceleration, numerical examples demonstrate that each solver shows distinct characteristics in terms of accuracy, computational efficiency and applicability.

1 Introduction

Full-wave numerical methods for computing electromagnetic fields inside inhomogeneous dielectric objects are typically based on differential or integral equations. Differential equation methods, such as finite element (FE) [1] and finite-difference frequency-domain (FDFD) [2] methods, discretize the wave equation in the computation domain with proper absorbing boundary conditions, and lead to sparse linear systems. In contrast, integral equation methods, such as volume integral equation (VIE) [3, 4, 5], volume surface integral equation [6, 7], and high-frequency asymptotic [8, 9] methods, rely on Green's function propagators without the need of artificial boundary conditions, and lead to dense linear systems. These sparse and dense systems can suffer from high-contrast ill-conditioning, high-frequency ill-conditioning, and/or numerical dispersion, and direct methods are often preferable. However, the computational costs of direct methods typically scale as $O(N^2)$ and $O(N^3)$ respectively for sparse and dense linear systems in 3D, where N is the number of degrees of freedom in the volume.

Many fast rank-structured direct solvers have been developed to model waves in inhomogeneous dielectrics. For sparse linear systems, multifrontal methods with low-rank hierarchical matrix representations [10, 11, 12] have been developed; for dense linear systems, \mathcal{H} matrices [13, 14], \mathcal{H}^2 matrices [15, 16, 17], and skeletonization [18, 19, 20] have been considered. The computational costs of these methods are shown to scale as $O(N)$ in the low- to medium-frequency regime. However, these low-rank based sparse

and dense linear solvers tend to be less efficient in the high-frequency settings. Recently, a new class of direct solvers based on the butterfly representation (see [21] and references therein), called hierarchically off-diagonal butterfly (HODBF) format [22], have been developed to show reduced complexities for surface integral equations (SIE) and have been extended to handle inhomogeneous dielectrics in high-frequency ranges. Examples include HODBF-based sparse multifrontal solvers for FE and FDFD systems [23], HODBF-based VIE solvers [24] and HODBF-based Babich SIE solvers [25]. Many of these solvers have been shown to scale quasi-linearly despite of the frequency range of interest. That said, their computational efficiency, accuracy and applicability are vastly different, and extra caution is required to choose the appropriate one in practice.

In this paper, we present some performance studies, including efficiency, accuracy and applicability, using the above-mentioned butterfly-based solvers for the computation of high-frequency electromagnetic fields inside an inhomogeneous dielectric object residing in 2D free space. Despite of efficiency/accuracy/applicability advantages of each solver, our numerical results show that: 1. the sparse FDFD solver suffers from numerical dispersion when at scale, and requires at least 50 points per wavelength (PPW) to achieve a reliable solution; 2. the VIE solver shows a complexity that is sub-optimal compared to the other solvers; 3. the Babich expansion-based solver requires smooth dielectric profiles that do not permit occurrence of caustics. These studies provide guidance on the choice of appropriate solver depending on the specific application need.

2 Butterfly-enhanced Direct Solvers for Inhomogeneous Dielectrics

For simplicity, we assume that an dielectric object with permittivity $\epsilon_r(\mathbf{r})$ and compact support V , residing in free space R^2 , is excited by an arbitrary time-harmonic source $s(\mathbf{r})$ outside V , with free space wave number k_0 . The fields inside V , $u(\mathbf{r})$, satisfy the Helmholtz equation:

$$[\nabla^2 + k_0^2 \epsilon_r(\mathbf{r})]u(\mathbf{r}) = -s(\mathbf{r}) \quad \text{in } R^2, \quad (1)$$

Next we summarize the three butterfly-enhanced direct methods for solving (1).

2.1 FDFD and sparse multifrontal solver

The FDFD method [2] discretizes (1) in the computation domain with perfectly matching layers, using $N_{fd} = n^2$ uniform Cartesian grids with 9-point finite-difference stencils. The resulting $N_{fd} \times N_{fd}$ sparse linear system is directly factorized using the butterfly-enhanced multifrontal solver [23]. Based on the fill-in reduction ordering, this solver generates a graph called the assembly tree to guide the LU factorization on the re-ordered matrix. Each node of the assembly tree corresponds to a dense frontal matrix, representing an intermediate dense submatrix in sparse Gaussian elimination. The factorization of the sparse matrix is cast into a series of partial factorizations and Schur complement updates of the frontal matrices. As the frontal matrices represent numerical Green's function interactions between the geometrical separators, large frontal matrices and their arithmetic operations are represented using the HODBF format [22]. The computational complexity of the resulting solver scales as $O(N_{fd})$. Despite of its optimal computational complexity and wide applicability, the FDFD solver suffers from numerical dispersion and requires high PPW to handle large-scale systems reliably. These features are summarized in Table 1.

Table 1. Performance summary of three butterfly-enhanced direct solvers for 2D electromagnetic analysis.

	FDFD	VIE	Babich-based SIE
System size to invert	$N_{fd} > N$	$N_v = N$	$N_s = O(N^{0.5})$
CPU time	$O(N)$	$O(N^{1.5} \log N)$	$O(N)$
PPW	>50	5-10	5-10
Permittivity	arbitrary	arbitrary	smooth

2.2 VIE method

The VIE converts (1) to an integral form

$$u(\mathbf{r}) = u^i(\mathbf{r}) + \int_V d\mathbf{r}' g_0(\mathbf{r}, \mathbf{r}') k_0^2 [\epsilon_r(\mathbf{r}') - 1] u(\mathbf{r}') \quad (2)$$

where u^i is the incident fields generated by source s , and $g_0(\mathbf{r}, \mathbf{r}')$ is the free-space Green's function. The VIE solver discretizes $u(\mathbf{r}')$ in V with $N_v = N$ piece-wise constant basis functions, leading to a dense $N \times N$ system. The butterfly-enhanced VIE solver [24] for 3D geometries compresses and inverts the system using the HODBF format. Here we apply it to the 2D setting of (1). Due to the need of inverting the large linear system, the computational cost of the butterfly-enhanced VIE solver scales sub-optimally as $O(N^{1.5} \log N)$ (see Table 1). That said, the VIE solver does not suffer from numerical dispersion (i.e. PPW=5-10 is sufficient), and applies to arbitrary dielectric profiles.

2.3 Babich expansion-based SIE method

For smooth analytic media that does not permit caustics, the Green's function can be directly constructed via the

Hadamard-Babich ansatz [25]:

$$g_{hb}(\mathbf{r}, \mathbf{r}') = \sum_{s=0}^{n_b} v_s(\mathbf{r}, \mathbf{r}') f_s(k_0, \tau), \quad (3)$$

$$f_s(k_0, \tau) = i \frac{\sqrt{\pi}}{2} e^{i s \pi} \left(\frac{2\tau}{k_0} \right)^s H_s^{(1)}(k_0 \tau). \quad (4)$$

Here, $H_s^{(1)}$ is the s -th Hankel function of the first kind, $v_s(\mathbf{r}, \mathbf{r}')$ and $\tau(\mathbf{r}, \mathbf{r}')$ are the amplitude and phase functions satisfying the transport equation and the eikonal equation with point source, respectively. Typically a two-term expansion with $n_b = 1$ is a good approximation of the true Green's function $g(\mathbf{r}, \mathbf{r}')$ for inhomogeneous media at high frequencies. In [25], the phase and amplitude functions τ , v_0 , v_1 are first tabulated by solving eikonal and transport equations with judiciously selected point sources. Once tabulated, they are fed into the butterfly compression algorithms for representing block-wise interactions via (3).

Here we extend its usage to modeling inhomogeneous dielectrics in free space. Similar to the SIE method to handle homogeneous dielectrics, here we replace the free-space Green's function in the interior domain with the Babich ansatz (3). Therefore one only need to discretize the ∂V with $N_s = O(N^{0.5})$ basis functions, leading to a dense $N_s \times N_s$ system whose HODBF-based inversion requires $O(N^{0.75} \log N)$ time. To compute fields everywhere inside V , the IE operator that maps equivalent source on ∂V to fields in V is also butterfly compressed, requiring $O(N)$ CPU time. Just like the VIE method, the Babich-based SIE method only requires PPW=5-10. That said, its applicability to general volumetric scatterers remains an open problem (See Table 1).

3 Numerical Results

In this section, we present one numerical example that demonstrates the accuracy and efficiency of the aforementioned butterfly-based solvers. The computation domain is $[0, 1]^2$ with background media $\epsilon_0 = 4$. The volumetric scatterer V is a square with side length 0.6 and center $[0.325, 0.325]$. The dielectric profile is $\epsilon_r(x, y) = (0.625 - 0.25y)^{-2}$ for $[x, y] \in V$. Note that $\epsilon_r(x, y)$ is analytical, hence all three solvers can be used here. The background wave number is set to $k_0 = 50\pi$, and accordingly the computation domain spans about 50 wavelengths in each direction. We consider two source functions, a point source $s(\mathbf{r}) = \delta(\mathbf{r}, \mathbf{r}_c)$ with $\mathbf{r}_c = [0.85, 0.85]$, and a Gaussian wavepacket source $s(\mathbf{r}) = \exp(-|\mathbf{r} - \mathbf{r}_c|^2 / (2\sigma^2)) \exp(ik_0(\mathbf{r} \cdot \mathbf{d}))$ with $\sigma = 0.15$ and $\mathbf{d} = \frac{1}{\sqrt{2}}[1, 1]$. The FDFD solver uses PPW=10 and 50, leading to linear systems of size $N_{fd} = 1,742,400$ and 43,560,000, respectively; the VIE solver uses PPW=10 leading to $N_v = 90,000$ volumetric unknowns; the Babich-SIE solver uses PPW=10 leading to $N_s = 2,400$ surface unknowns. All solvers leverage the HODBF format supported in the open-source software package ButterflyPACK [26]. All tests are performed on the Haswell nodes of the Cori machine, a Cray XC40, at NERSC in Berkeley.

The fields computed by the three solvers are shown in Figure 1 (a)-(b). It is clear that the wavelength becomes shorter at y increases inside V . Figure 1 (c)-(d) demonstrates that the FDFD solver requires at least PPW=50 for the solution to agree well with those of the VIE and Babich-SIE solvers, which only require PPW=10. In addition to the accuracy comparison, it's worth mentioning that the system inversion in the VIE and Babich-SIE solvers are quite fast due to their compact sizes. That said, we expect that the VIE timing will degrade for much larger sized systems according to complexity estimates in Table 1. Moreover, if one is interested in computation of the farfields instead of fields inside V , the Babich-SIE solver is the fastest (i.e., $O(N^{0.75} \log N)$) among all three solvers.

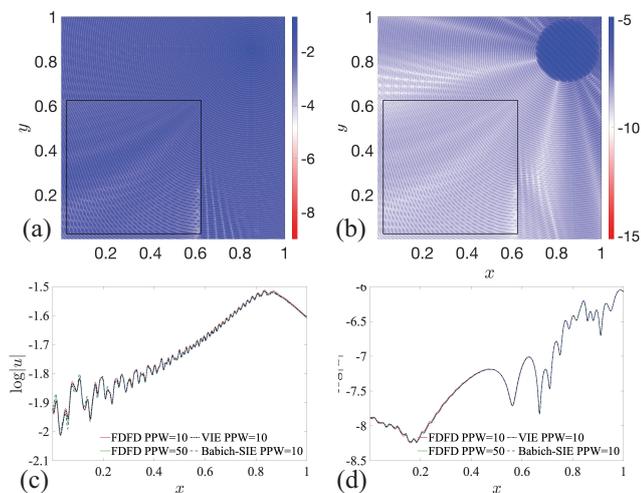


Figure 1. (a-b): Wavefields u in the computation domain with an inhomogeneous dielectric in $[0.025, 0.625]^2$ (marked by the black boundary lines) generated by (a) the point source and (b) the Gaussian wavepacket source. (c)-(d): Accuracy comparison of the three butterfly-based solvers: FDFD with PPW=10 and 50, VIE with PPW=10 and Babich-SIE with PPW=10, with fields along $y = 0.99$ generated from (c) the point source and (d) the Gaussian wavepacket source.

4 Conclusion

We present a preliminary performance study of three butterfly-enhanced direct solvers, namely FDFD, VIE and Babich-SIE, for analyzing high-frequency electromagnetic phenomena involving inhomogeneous dielectrics. Despite of their favorable computational complexities, the FDFD solver requires large PPW to compensate for numerical dispersion; the VIE solver requires asymptotically the most expensive computation due to the inversion of large systems; the Babich-SIE solvers requires the dielectrics to be smooth and simple. All these constraints need extra caution for practitioners interested in full-wave simulation of large-scale inhomogeneous dielectrics.

5 Acknowledgements

This research was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program through the FAST-Math Institute under Contract No. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

References

- [1] J. Jin, "The finite element method in electromagnetics," 2014.
- [2] Z. Chen, D. Cheng, W. Feng, and T. Wu, "An optimal 9-point finite difference scheme for the helmholtz equation with pml." *International Journal of Numerical Analysis & Modeling*, vol. 10, no. 2, 2013.
- [3] 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.
- [4] M. Sancer, K. Sertel, J. Volakis, and P. VanAlstine, "On volume integral equations," *IEEE Trans. Antennas Propag.*, vol. 54, no. 5, pp. 1488–1495, may 2006.
- [5] M. M. Botha, "Solving the volume integral equations of electromagnetic scattering," *J. Comput. Phys.*, vol. 218, no. 1, pp. 141–158, oct 2006.
- [6] B. Usner, K. Sertel, M. Carr, and J. Volakis, "Generalized volume-surface integral equation for modeling inhomogeneities within high contrast composite structures," *IEEE Transactions on Antennas and Propagation*, vol. 54, no. 1, pp. 68–75, 2006.
- [7] L. J. Gomez, A. C. Yücel, and E. Michielssen, "The icvsie: a general purpose integral equation method for bio-electromagnetic analysis," *IEEE Transactions on Biomedical Engineering*, vol. 65, no. 3, pp. 565–574, 2017.
- [8] J. Qian, L. Yuan, Y. Liu, S. Luo, and R. Burrige, "Babich's expansion and high-order eulerian asymptotics for point-source helmholtz equations," *Journal of Scientific Computing*, vol. 67, no. 3, pp. 883–908, 2016.
- [9] W. Lu, J. Qian, and R. Burrige, "Extending babich's ansatz for point-source maxwell's equations using hadamard's method," *Multiscale Modeling & Simulation*, vol. 16, no. 2, pp. 727–751, 2018.

- [10] P. Ghysels, X. S. Li, C. Gorman, and F.-H. Rouet, "A robust parallel preconditioner for indefinite systems using hierarchical matrices and randomized sampling," in *2017 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, 2017, pp. 897–906.
- [11] P. Amestoy, C. Ashcraft, O. Boiteau, A. Buttari, J.-Y. L'Excellent, and C. Weisbecker, "Improving multifrontal methods by means of block low-rank representations," *SIAM J. Sci. Comput.*, vol. 37, no. 3, pp. A1451–A1474, 2015.
- [12] B. Zhou and D. Jiao, "Direct Finite-Element Solver of Linear Complexity for Large-Scale 3-D Electromagnetic Analysis and Circuit Extraction," *IEEE T. MICROW. THEORY*, vol. 63, no. 10, pp. 3066–3080, 2015.
- [13] R. Gholami, J. Mojolagbe, A. Menshov, F. S. Hosseini Lori, and V. I. Okhmatovski, " \mathcal{H} -matrix arithmetic for fast direct and iterative method of moment solution of surface-volume-surface EFIE for 3-D radiation problems," *Progress In Electromagnetics Research*, vol. 82, pp. 189–210, 2018.
- [14] R. Gholami and V. Okhmatovski, "Surface-volume-surface EFIE formulation for fast direct solution of scattering problem on general 3-D composite metal-dielectric objects," *IEEE Trans. Antennas Propag.*, 2020.
- [15] S. Omar and D. Jiao, "A linear complexity direct volume integral equation solver for full-wave 3-D circuit extraction in inhomogeneous materials," *IEEE Trans. Microwave Theory Tech.*, vol. 63, no. 3, pp. 897–912, 2015.
- [16] M. Ma and D. Jiao, "Accuracy directly controlled fast direct solution of general matrices and its application to solving electrodynamic volume integral equations," *IEEE Trans. Microwave Theory Tech.*, vol. 66, no. 1, pp. 35–48, 2017.
- [17] —, "Direct solution of general \mathcal{H} -matrices with controlled accuracy and concurrent change of cluster bases for electromagnetic analysis," *IEEE Trans. Microwave Theory Tech.*, vol. 67, no. 6, pp. 2114–2127, 2019.
- [18] L. Greengard, D. Gueyffier, P.-G. Martinsson, and V. Rokhlin, "Fast direct solvers for integral equations in complex three-dimensional domains," *Acta Numerica*, vol. 18, pp. 243–275, 2009.
- [19] E. Corona, P.-G. Martinsson, and D. Zorin, "An $O(N)$ direct solver for integral equations on the plane," *Appl. Comput. Harmon. Anal.*, vol. 38, no. 2, pp. 284 – 317, 2015.
- [20] Y.-N. Liu, X.-M. Pan, and X.-Q. Sheng, "Fast direct solution of 3-D volume integral equations by skeletonization for dynamic electromagnetic wave problems," *International Journal of Numerical Modelling: Electronic Networks, Devices and Fields*, vol. 33, no. 2, p. e2667, 2020.
- [21] Y. Liu, X. Xing, H. Guo, E. Michielssen, P. Ghysels, and X. S. Li, "Butterfly factorization via randomized matrix-vector multiplications," *SIAM Journal on Scientific Computing*, vol. 43, no. 2, pp. A883–A907, 2021.
- [22] Y. Liu, H. Guo, and E. Michielssen, "An hss matrix-inspired butterfly-based direct solver for analyzing scattering from two-dimensional objects," *IEEE Antennas Wireless Propag. Lett.*, vol. 16, pp. 1179–1183, 2016.
- [23] Y. Liu, P. Ghysels, L. Claus, and X. S. Li, "Sparse approximate multifrontal factorization with butterfly compression for high-frequency wave equations," *SIAM Journal on Scientific Computing*, no. 0, pp. S367–S391, 2021.
- [24] S. B. Sayed, Y. Liu, L. J. Gomez, and A. C. Yucel, "A butterfly-accelerated volume integral equation solver for broad permittivity and large-scale electromagnetic analysis," *IEEE Transactions on Antennas and Propagation*, 2021.
- [25] Y. Liu, J. Song, R. Burrige, and J. Qian, "A fast butterfly-compressed hadamard-babich integrator for high-frequency helmholtz equations in inhomogeneous media with arbitrary sources," *submitted to Multiscale Modeling & Simulation*.
- [26] <https://github.com/liuyangzhuang/ButterflyPACK>.