VoxCap: FFT-Accelerated and Tucker-Enhanced Capacitance Extraction Simulator for Voxelized Structures

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Abstract—VoxCap, a fast Fourier transform (FFT)-accelerated and Tucker-enhanced integral equation simulator for capacitance extraction of voxelized structures, is proposed. The VoxCap solves the surface integral equations (SIEs) for conductor and dielectric surfaces with three key attributes that make the VoxCap highly CPU and memory efficient for the capacitance extraction of the voxelized structures: (i) VoxCap exploits the FFTs for accelerating the matrix-vector multiplications during the iterative solution of linear system of equations arising due to the discretization of SIEs. (ii) During the iterative solution, VoxCap uses a highly effective and memory-efficient preconditioner that reduces the number of iterations significantly. (iii) VoxCap employs Tucker decompositions to compress the block Toeplitz and circulant tensors, requiring the largest memory in the simulator. By doing so, it reduces the memory requirement of these tensors from hundreds of gigabytes to a few megabytes and the CPU time required to obtain Toeplitz tensors from tens of minutes (even hours) to a few seconds for very large scale problems. VoxCap is capable of accurately computing capacitance of arbitrarily shaped and large-scale voxelized structures on a desktop computer. VoxCap’s accuracy, efficiency, and capability are demonstrated through capacitance extraction of various large-scale structures, including the parallel meander lines discretized by more than a hundred million panels and analyzed on a commodity desktop computer.

Index Terms—Capacitance extraction, electrostatic analysis, fast Fourier Transform (FFT), fast simulators, Tucker decomposition, surface integral equation (SIE), voxelized structures.

I. INTRODUCTION

Recent developments in three-dimensional (3D) printing technology have allowed the designers to produce their own prototypes conveniently and reduce the prototype development time dramatically. Today’s 3D printers build the integrated circuits/packages/components voxel by voxel (i.e., cube by cube). Therefore, virtual fabrication environments leveraging voxels have recently been received significant traction. By using these environments, the designers can iteratively explore their designs; they can alter their designs and check whether their designs meet certain design specifications. During this iterative process, the designers are in need of fast and accurate parameter extraction simulators that can be used in conjunction with virtual fabrication environments and operated on circuits/structures discretized by voxels (i.e., voxelized structures). Unfortunately, the current literature does not have enough studies on the development of such simulators: An inductance extraction simulator for voxelized structures, called VoxHenry [1], was recently proposed. That said, there exists no study on the capacitance extraction for the voxelized structures so far.

The literature abounds with the capacitance extraction simulators based on finite-difference [2-4], finite-element [5-7], integral equation [8-16] methods. While these methods are no panacea, none of them is developed for / directly applicable to the voxelized structures and can readily extract capacitances by only using the voxel coordinates provided from the virtual fabrication environment. When used for voxelized structures, all current simulators require the users’ intervention such as the inclusion of artificial absorbing boundaries or generation of complicated mesh. Furthermore, none of the integral equation simulators is developed by exploiting the distinct features arising from the structured grid of voxelized structure. Aside from these, those cannot be easily coupled with the VoxHenry to extract impedances of the voxelized structures. To this end, a capacitance extraction simulator that can exploit all distinct features of voxelized structures, be used in conjunction with voxel-based virtual fabrication environments without users’ intervention, and be easily coupled with the VoxHenry simulator is called for.

In this study, a capacitance extraction simulator for voxelized structures, called VoxCap, is proposed. The VoxCap solves the surface integral equations (SIEs) for the conductor and dielectric surfaces after discretizing the charges on these surfaces via piecewise constant basis functions and obtaining a linear system of equations (LSE) via Galerkin testing. It leverages the following three features, which make the VoxCap highly CPU and memory-efficient while solving the LSE and obtaining the capacitances of voxelized structures:
1. The VoxCap exploits the fast Fourier transforms (FFTs) to accelerate the matrix-vector multiplications (MVMs) during the iterative solution of LSE.

2. The VoxCap uses an effective and memory-efficient block-diagonal-diagonal preconditioner to ensure the fast convergence of the iterative solution.

3. The VoxCap leverages Tucker decompositions to dramatically reduce the memory requirement of the block circulant tensors as well as the CPU time required to obtain Toeplitz tensors.

All these features make the contribution of this study threefold, as described below. The FFTs have been widely applied to integral equation simulators to accelerate the MVMs by exploiting the translationally-invariance property of the integral kernels sampled on the structured grids [1, 17-20]. Although it was applied to the 2D static problems in [21], there exists no study providing the implementation of the FFT acceleration for the capacitance extraction of 3D voxelized structures in the literature, to the best of our knowledge. Along with the FFT accelerations, a memory efficient preconditioning technique hybridizing block-diagonal and diagonal preconditioners is proposed in this study by showing its effectiveness compared to those of traditional diagonal and block-diagonal preconditioners. Moreover, Tucker decompositions are proposed for the first time in this study to compress the block circulant and Toeplitz tensors of static integral kernels, which require the largest memory in the simulator. The proposed Tucker decomposition reduces the memory requirement of these tensors more than four orders of magnitude (from tens/hundreds of gigabytes to megabytes). The Tucker-compressed Toeplitz tensors are obtained once and for all and stored on hard-disk during the installation stage of the simulator. During the setup stage of each execution of the VoxCap, the compressed Toeplitz tensors are read from the hard disk in seconds, resized/updated by accounting for the sizes of computational domain and voxels, and used to obtain the block circulant tensors. Doing so reduces the setup stage of the proposed simulator from tens of minutes (even hours) to a few seconds for large-scale problems. During the iterative solution stage of the VoxCap, the compressed circulant tensors are restored/decompressed to their original format one-by-one and used in MVMs. Doing so significantly reduces the overall memory cost of the proposed simulator while imposing negligible computational overhead arising from the restoration/decompression operation.

The accuracy and efficiency of the proposed VoxCap simulator are demonstrated (and compared with FastCap [15] when applicable) through its application to the capacitance extraction of various structures including a dielectric-coated perfect electric conductor (PEC) sphere, a PEC cube, a parallel interconnect structure, and a parallel meander line structure. The capability of the VoxCap simulator for solving very large-scale problems on a desktop computer is shown by its application to the capacitance extraction of a very large-scale parallel meander line structure discretized by more than one hundred million panels. Moreover, the memory saving achieved by and computational overhead imposed by the Tucker enhancement are extensively quantified for 3D and 2D-like structures. The numerical results show that the proposed VoxCap outperforms the FastCap for many practical scenarios comprising densely packed interconnects. In particular, the VoxCap requires 15x and 30x less memory as well as 2.5x and 5x less CPU time compared to FastCap for the same level of accuracy in the analyses of parallel interconnect structure and parallel meander line structure, respectively. For the analysis of dielectric-coated cube discretized by 400 voxels along x-, y-, and z-directions, the Tucker enhancement reduces the memory requirement of the circulant tensors more than 10,000x while imposing a negligible computational overhead, one-sixth of the CPU time required for one convolution. For the same problem, the Tucker enhancement allows achieving more than 4655x speed-up for obtaining the Toeplitz tensors. Moreover, the scaling of the memory requirement of the Tucker-compressed tensors with respect to increasing computational domain size is found to be sub-linear, while that of the memory requirement of the original circulant and Toeplitz tensors are linear. It should be noted here that the proposed VoxCap simulator is elaborated for the first time in this paper. The presentation, which sketches the basic principles of the simulator, has been given at an earlier symposium [22].

II. FORMULATION

In this section, the SIEs solved by VoxCap, their discretization, and resulting LSE are explained first. Next, the implementation details of the FFTs for the MVMs required during the iterative solution of LSE are provided. Then the proposed preconditioner for reducing the number of iterations during the iterative solution of LSE is described. Finally, the proposed Tucker decomposition/compression scheme is expounded.

A. SIEs and Their Discretization

Let $S_c$ and $S_d$ denote PEC and dielectric surfaces with the charge densities $\sigma$ and $\sigma_d$, respectively [Fig. 1(a)]. The dielectric surface with outward normal $\hat{n}_d$ separates the dielectric region with permittivity $\varepsilon_d$ from the background medium with permittivity $\varepsilon_0$. The PEC and dielectric surfaces are assumed to be enclosed by a bounding box [Fig. 1(b)] that consists of $N_v$ voxels with the edge size $\Delta v$; $N_i = N_x \times N_y \times N_z$, where $N_x$, $N_y$, and $N_z$ denote the number of voxels along x-, y-, and z-directions, respectively. In this setting, the capacitance of the structure is computed by solving SIEs [23], which read

$$\Phi(r) = \int_{S_c} \sigma(r') G(r, r') dS' + \int_{S_d} \sigma_d(r') G(r, r') dS', \quad r \in S_c \quad (1)$$

$$\varepsilon_0 \frac{\partial \Phi'(r)}{\partial n_j} = \varepsilon_d \frac{\partial \Phi'(r)}{\partial n_j}, \quad r \in S_d \quad (2)$$

where $G(r, r') = 1/(4\pi \varepsilon_0 |r - r'|)$ is the free-space Green’s function, $r$ and $r'$ denote the observer and source points on the surfaces, respectively, and $\varepsilon_0$ is the permittivity of free space. While $\Phi(r)$ denotes the potential on the surface, $\Phi'(r)$ and $\Phi(r)$ represent the potentials while approaching to the...
surface from dielectric and background media, respectively. To solve (1) and (2), $\sigma_i$ and $\sigma_j$ are discretized using the piecewise constant basis functions $w_i$ defined on $N_i$ conductor and $N_j$ dielectric panels as

$$\sigma_i(r') \equiv \sum_{i=1}^{N_i} w_i(r') \rho_{i,j}, \quad \sigma_j(r') \equiv \sum_{j=1}^{N_j} w_i(r') \rho_{i,j}, \quad (3)$$

where $w_i(r') = 1$ for $r' \in S_i$; $w_i(r') = 0$, otherwise. $S_i$ denotes the surface of $l$th panel and $\rho_{i,j}$ and $\rho_{j,i}$ are the unknown coefficients of the charge density on the PEC and dielectric panels, respectively. Substituting (3) into (1)-(2), applying Galerkin testing to the resulting equations with $w_i(r')$, $k = 1, \ldots, N_i$, and evaluating limits for (2) when $l = k$ [24] yields an $N \times N$ LSE as ($N = N_i + N_j$)

$$\left[ \begin{array}{c} V \\ 0 \end{array} \right] = \left( \begin{array}{c} 0 \\ I + \mathbf{P} \end{array} \right) \left[ \begin{array}{c} \rho_i \\ \rho_j \end{array} \right], \quad (4)$$

where $\rho_i = [\rho_{i,1}, \rho_{i,2}, \ldots, \rho_{i,N}], \rho_j = [\rho_{j,1}, \rho_{j,2}, \ldots, \rho_{j,N}]$ are the charge coefficient vectors, $\mathbf{P}$ and $\mathbf{E}$ matrices with dimensions $N_i \times N$ and $N_j \times N$ relate the potentials and electric fields tested on the panels with the charges, respectively. The entries of $\mathbf{P}_{ij}$, $k = 1, \ldots, N_i$, $l = 1, \ldots, N_j$ are

$$\mathbf{P}_{ij} = \int_{S_i} \int_{S_j} w_i(r) w_j(r') G(r, r') dS dS, \quad (5)$$

and those of $\mathbf{E}_{ij}$ and diagonal matrix $I_{ij}$, $k = 1, \ldots, N_i$, $k' = k + N_i$, $l = 1, \ldots, N_j$ are obtained for non-overlapping and overlapping panels, respectively, via

$$\mathbf{E}_{ij} = \frac{\partial}{\partial n_i} \int_{S_i} \int_{S_j} w_i(r) w_j(r') G(r, r') dS dS, \quad (6)$$

$$I_{ii} = (A_i (e_{j} + e_{j'}) - (2 e_0 (e_{j} - e_{j'}))) \quad (7)$$

where $A_i$ and $\partial / \partial n_i$ represent the area of $S_i$ and partial derivative along the normal to $S_i$, respectively. $V_i = A_i \Phi_i$, $k = 1, \ldots, N_i$. $\Phi_i$ is the potential applied to the panel on the conductors. For near panel interactions, the integrals in (5) and (6) are evaluated via analytical formulae in Appendix C of [25] and Appendix A, respectively. For far panel interactions, those integrals are evaluated using numerical quadrature and differentiation [24].

To compute the self and mutual capacitances of $m$ conductors, a unit potential is applied to each conductor separately while the potential of the remaining conductors is set to zero, and the LSE in (4) is solved for charge densities. The resulting $m$ number of $V$ and $\rho$ vectors are stored in matrices as $\mathbf{V} = [V^1, V^2, \ldots, V^m]$ and $\mathbf{P}_i = [\rho_i^1, \rho_i^2, \ldots, \rho_i^m]^T$, which are then used to compute $m \times m$ capacitance matrix $\mathbf{C}$ as

$$\mathbf{C} = \mathbf{V} \mathbf{P}_i^{-1} \mathbf{V}^T. \quad (8)$$

For the conductor embedded in a dielectric medium, its surface charge is converted to free charge density by multiplying it with $\varepsilon_d / \varepsilon_0$ and used in (8) [24].

The LSE in (4) is iteratively solved for $\rho_i$ and $\rho_j$ via a sequence of MVMs. During the iterative solution, the computational cost of MVMs and the memory requirement of the system matrices scale with $O(N^2)$; the former and the latter are reduced to $O(N \log N_i)$ and $O(N_i)$, respectively, via the FFT method explained next. Such computational cost and memory requirements are highly favorable for the capacitance extraction of the densely packed interconnects [16].

![Fig. 1. An example scenario: (a) A structure consisting of interconnects in a dielectric substrate and (b) its discretization via voxels.](image)

**B. FFT Acceleration**

In the FFT acceleration technique, the multiplications of matrices $\mathbf{P}$ and $\mathbf{E}$ vectors are stored in $\mathbf{P}_i$ and $\mathbf{E}_i$, respectively, via group panel interactions with respect to their unit normal as

$$\mathbf{V}^* = \left[ \begin{array}{c} 0 \\ I \end{array} \right] \left[ \begin{array}{c} \mathbf{P}_i \mathbf{E}_i \end{array} \right] \left[ \begin{array}{c} \mathbf{P}_i \mathbf{P}_j \end{array} \right], \quad \mathbf{P}^* = \left[ \begin{array}{c} 0 \\ I \end{array} \right] \left[ \begin{array}{c} \mathbf{P}_i \mathbf{E}_i \end{array} \right] \left[ \begin{array}{c} \mathbf{P}_i \mathbf{P}_j \end{array} \right], \quad (9)$$

where $\mathbf{P} = [\rho_i^1; \rho_j^1], \mathbf{P}^* = [\rho_i^1; \rho_j^1], \mathbf{P}^* = [\rho_i^1; \rho_j^1]$ are the vectors of the charge coefficients of the panels with unit normal pointing along $x$, $y$, and $z$-directions. Here the block matrix $\mathbf{V}^*$, for example, stores the potentials generated by the charges on the panels with unit normal pointing along $x$-direction and tested on panels with unit normal pointing along the $y$-direction. The full block matrices are multiplied with charge coefficient vectors as

$$\mathbf{C}^\alpha = \sum_\beta \mathbf{P}_i^\alpha \mathbf{P}_j^\beta, \quad \mathbf{D}^\alpha = \sum_\beta \mathbf{E}_i^{\alpha, \beta} \mathbf{P}_j^\beta \quad (10)$$

where $\alpha, \beta \in \{x, y, z\}$. Note that the multiplications of $\mathbf{P}^\alpha$ with the diagonal matrix $I$ in (9) are computationally cheap and performed traditionally. However, the multiplications of $\mathbf{E}^\alpha$ with the full block matrices $\mathbf{P}_i^{\alpha, \beta}$ and $\mathbf{E}_i^{\alpha, \beta}$ are computationally expensive and thereby accelerated via FFT technique. In this technique, the multiplications are performed by taking into account the panels of $N_i$ voxels instead of $N$ boundary panels on the PEC and dielectric surfaces. To do that, first, $(N_i + 1) \times N_i \times N_i$, $N_i \times (N_i + 1) \times N_i$, and $N_i \times N_j \times (N_i + 1)$ numbers of voxel panels with unit normal pointing along $x$, $y$, and $z$-directions are identified, respectively. These voxel panels lie on structured grids and
thereby their interactions are characterized by block Toeplitz tensors. The block Toeplitz tensors $A^{\alpha,\beta}$ and $B^{\alpha,\beta}$ are used to obtain block circulant tensors $P^{\alpha,\beta}$ and $E^{\alpha,\beta}$ corresponding to blocks $F^{\alpha,\beta}$ and $E^{\alpha,\beta}$, $\alpha, \beta \in \{x, y, z\}$. The procedure to obtain the block Toeplitz tensors and the circulant tensors are explained in Appendix B. The block circulant tensors are Fourier transformed and stored as $\hat{P}^{\alpha,\beta}$ and $\hat{E}^{\alpha,\beta}$ during the setup stage of the simulator. During the iterative solution stage, they are used to perform the MVMs corresponding to each block as

$$C^\alpha = \text{IFFT} \left\{ \sum_\beta \hat{P}^{\alpha,\beta} \hat{Q}^\beta \right\}, \quad D^\alpha = \text{IFFT} \left\{ \sum_\beta \hat{E}^{\alpha,\beta} \hat{Q}^\beta \right\},$$

(11)

where $\hat{}$ denotes the tensor-tensor multiplication, $\text{IFFT}\{\}$ is the inverse FFT operator, and $\hat{Q}^\beta = \text{FFT}\{Q^\beta\}$. The tensor $Q^\beta$ with the dimensions $2(N_i+1) \times 2(N_i+1) \times 2(N_i+1)$ is filled by the samples from $p^\beta$ and zeros [26]. The results of MVMs, $C^\alpha$ and $D^\alpha$, are obtained from the entries of $C^\alpha$ and $D^\alpha$.

A couple of notes regarding the computation of circulant tensors and their deployment in FFT operations are in order:

1) Although the dimensions of each circulant tensor vary due to the different numbers of voxel panels aligned along $x$-, $y$-, and $z$-directions, the dimensions of all circulant tensors are enlarged to $2(N_i+1) \times 2(N_i+1) \times 2(N_i+1)$ by carefully padding zeros, as explained in Appendix B. Such zero-padding enables to reduce the number of FFT operations from nine to three while computing $\hat{Q}^\beta$ and the number of IFFT operations from nine to three while computing each of $C^\alpha$ and $D^\alpha$, $\alpha \in \{x, y, z\}$.

2) By exploiting the symmetry and invoking the properties of Fourier transform [21], some of the FFT-ed circulant tensors are obtained from others via complex conjugation as $\hat{P}^{\alpha,-i} = \text{conj}\{\hat{P}^{\alpha,i}\}$, $\hat{P}^{\alpha,-r} = \text{conj}\{\hat{P}^{\alpha,r}\}$, $\hat{P}^{\alpha,-\gamma} = \text{conj}\{\hat{P}^{\alpha,\gamma}\}$. Doing so allows reducing the memory footprint of the simulator, the Toeplitz tensors $A^{\alpha,\beta}$ and $B^{\alpha,\beta}$ are computed for a large computational domain (say $N_x = N_y = N_z = 1,000$) by setting $\Delta v = 1 \text{ m}$, compressed by Tucker decompositions, and stored on the hard disk. During the setup stage of each execution, the compressed tensors requiring megabytes of memory are read from the hard disk and restored to their original format. The restored Toeplitz tensors are resized with respect to the dimensions of the computational domain required for the structure being analyzed. Next, the restored Toeplitz tensors are multiplied with scaling factors related to the voxel size. These scaling factors, derived in Appendix C, are $(\Delta v)^3$ and $(\Delta v)^2$ for $A^{\alpha,\beta}$ and $B^{\alpha,\beta}$, respectively.

3) The directions of the panels’ unit normal should be carefully taken into account while obtaining the entries of $D^\alpha$ from $D^\alpha$. The entries of $D^\alpha$ for boundary panels with unit normal pointing along positive $x$-, $y$-, and $z$-directions are directly retrieved from the entries of $D^\alpha$, whereas those for boundary panels with unit normal pointing along negative $x$-, $y$-, and $z$-directions are obtained from the entries of $D^\alpha$ after flipping the signs of entries.

C. Tucker Enhancement

The proposed VoxCap simulator uses Tucker decompositions to compress the Toeplitz tensors $A^{\alpha,\beta}$ and $B^{\alpha,\beta}, \alpha, \beta \in \{x, y, z\}$, once and for all during the installation stage. During the setup stage of the simulator’s execution, the compressed Toeplitz tensors are read from the hard disk and used to obtain the circulant tensors. Doing so allows reducing the setup stage time of the simulator from tens of minutes (and even hours) to seconds, as shown in Table I of Section III.C.3. To do that, during the installation stage of the simulator, the Toeplitz tensors $A^{\alpha,\beta}$ and $B^{\alpha,\beta}$ are used in the embedding procedure explained in Appendix B to obtain circulant tensors.

In addition, the proposed VoxCap simulator leverages Tucker decompositions to reduce the memory requirement of the FFT’ed circulant tensors $\hat{P}^{\alpha,\beta}$ and $\hat{E}^{\alpha,\beta}, \alpha, \beta \in \{x, y, z\}$. Doing so allows reducing the memory footprint of the simulator around a factor of three and half for the capacitance extraction of dielectric coated PEC structures and a factor of two for the capacitance extraction of PEC structures, as shown in numerical examples in Section III.A and III.B. To do that, during the setup stage of the simulator, all $\hat{P}^{\alpha,\beta}$ and $\hat{E}^{\alpha,\beta}, \alpha, \beta \in \{x, y, z\}$ are compressed by Tucker decomposition. During the iterative solution stage, each compressed tensor is restored/decompressed to its original format one-by-one. The computational penalty associated with the restoration operation is negligible compared to one convolution operation perform during MVMs, as shown in the numerical results section.

The Toeplitz and FFT’ed circulant tensors are compressed by Tucker decompositions as [20, 27-29]

$$\mathbf{X} \approx S \times_1 \tilde{U}_1 \times_2 \tilde{U}_2 \times_3 \tilde{U}_3,$$

(13)

where the tensor $\mathbf{X}$ with dimensions $D_1 \times D_2 \times D_3$ represents $A^{\alpha,\beta}, B^{\alpha,\beta}, \hat{P}^{\alpha,\beta}$, or $\hat{E}^{\alpha,\beta}, \alpha, \beta \in \{x, y, z\}$, $S$ is the core tensor with dimensions $r_1 \times r_2 \times r_3$, $\tilde{U}_i, i = 1, \ldots, 3$, represents the factor matrices with dimensions $D_i \times r_i$, and $r_i$ is the

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**Algorithm 1** Procedure to obtain core tensor and factor matrices

1. Obtain three mode-$i$ unfolding matrices of $\mathbf{X}$, denoted by $\mathbf{X}_i, i=1,\ldots,3$
2. Compute singular value decompositions of $\mathbf{X}_i = \mathbf{U}_i \mathbf{\Sigma}_i \mathbf{V}_i^*$, $i=1,\ldots,3$
3. Find the indices of maximum (normalized) singular values in $\mathbf{\Sigma}_i$, $i=1,\ldots,3$, smaller than tolerance $tol/\sqrt{3}$ and assign those to $r_i, i=1,\ldots,3$
4. Truncate the left singular vectors $\mathbf{U}_i$ with $r_i, i=1,\ldots,3$
5. Obtain the core tensor via $S = \mathbf{X}_1 \mathbf{U}_1^\top \times_2 \mathbf{U}_2^\top \times_3 \mathbf{U}_3^\top$.
multilinear rank pertinent to \( i^{th} \) dimension. A tensor is Tucker compressible in case \((r_1r_2) + \sum \lambda_i D^r_i < r D_1 D_2 \). The symbol \( x_i \), \( i=1,...,3 \), stands for \( i \)-mode matrix-tensor multiplication, which can be performed for the 1st dimension in (13) as an example:

\[
\mathbf{Y}_{v, v} = S_{x_i} \mathbf{U}^i = \sum_{r, t} S_{x_i x_r} \mathbf{U}^i_{x_r}
\]

(14)

where \( \mathbf{Y}_{v, v} \) is the resulting tensor with indices \( v_1=1,...,D_t \), \( v_2=1,...,r_2 \), and \( v_3=1,...,r_3 \). The procedure to obtain the \( S \) and \( \mathbf{U}^i \) for given tolerance, \( t o l \), is provided in Algorithm 1. Typically, \( t o l \) is set to \( 10^{-6} \) in this study to achieve high compressibility without sacrificing from the accuracy, unless stated otherwise. In Algorithm 1, the unfolding matrices of a tensor can be readily obtained by reshaping operations [30].

D. Block-Diagonal-Diagonal Preconditioner

The proposed VoxCap simulator uses a block-diagonal-diagonal preconditioner to ensure the rapid convergence of the iterative solution of (4). To this end, during each MVM, the block diagonal preconditioner \( \mathbf{R}_{BD} \) and diagonal preconditioner \( \mathbf{R}_{D} \) are applied to (4) as

\[
\begin{bmatrix}
\mathbf{R}_{BD}

\end{bmatrix}
\begin{bmatrix}
\mathbf{V}

\end{bmatrix} = \begin{bmatrix}
\mathbf{R}_{BD}

\end{bmatrix} \begin{bmatrix}
0

\end{bmatrix} + \begin{bmatrix}
\mathbf{F}

\end{bmatrix} \begin{bmatrix}
\rho

\end{bmatrix}
\]

(15)

The entries of the diagonal matrix \( \mathbf{R}_{D} \) are directly obtained from the inverse of the diagonal matrix \( \mathbf{I}_{D} \). The blocks of block-diagonal matrix \( \mathbf{R}_{BD} \) are formed by (i) splitting the bounding box enclosing the structure into small boxes, (ii) computing the interactions between basis functions in each small box separately, and (iii) assigning the inverses of the submatrices storing the interactions as blocks of \( \mathbf{R}_{BD} \). Each small box comprises of \( N_{\alpha} \), \( N_{\beta} \), and \( N_{\gamma} \) voxels along \( x \)-, \( y \)-, and \( z \)-directions. For an example PEC interconnect scenario, this partitioning and the basis functions/panels used to form the blocks are shown in Fig. 2 (\( N_{\alpha} = N_{\beta} = 16 \) and \( N_{\gamma} = 1 \)). Two important points regarding to the construction and storage of the blocks are in order: (i) The interactions between basis functions in each small box are directly obtained from one-time generated circulant tensors \( \mathbf{P}^{x, \beta} \) and \( \mathbf{E}^{y, \beta} \), \( \alpha, \beta \in \{x, y, z\} \) for a small box consisting of \( N_{\alpha} \), \( N_{\beta} \), and \( N_{\gamma} \) voxels. This yields significant computational saving while constructing the preconditioner. Note that the circulant tensors store all possible basis function interactions for a small box. By using these tensors, the computational time required to compute (5) for similar basis function pairs in blocks are avoided. (ii) Many blocks in \( \mathbf{R}_{BD} \) are the replicates of each other for a voxelized structure. To this end, only one block is stored and the memory requirement of the preconditioner is minimized.

III. NUMERICAL RESULTS

In this section, several numerical examples that show the applicability, memory and CPU efficiency, and accuracy of the proposed VoxCap simulator are presented. In the following analysis, when applicable, the capacitance values obtained by VoxCap and FastCap are compared with each other or those obtained by an analytical formula. The discrepancy between the results is quantified through the relative error defined as

\[
\text{err}(\epsilon) = \left\| (F - \tilde{F}) / \tilde{F} \right\|,
\]

where \( F \) and \( \tilde{F} \) denote the capacitance values obtained by VoxCap/FastCap and analytical formula, respectively. Furthermore, the charge distributions on the structures are plotted in the logarithmic (dB) scale after all charge values are normalized by the maximum charge value on the structure and the logarithm of normalized values are multiplied by twenty. The proposed VoxCap simulator was implemented in Matlab, while the FastCap simulator executes a C code. The linear system of equations in Eqn. (4) is iteratively solved by generalized minimal residual method (GMRES) with a restart every 35 iterations until the relative residual error (RRE) reaches to \( 10^{-7} \), unless stated otherwise. All simulations are executed on an Intel Xeon Gold 6412 CPU with 384 GB RAM.

A. The Dielectric-Coated PEC Sphere

First, the proposed VoxCap simulator and FastCap simulator (with 4th order multipole expansion) are used to obtain the self-capacitance of a 0.25 m - radius PEC sphere coated by a dielectric shell with relative permittivity \( \epsilon \) and radius of 0.5 m [Fig. 3(a)]. The structure is discretized by voxels of size \( \Delta r = [0.05, 0.025, 0.02, 0.01] \) m, which gives rise to \( N_{\alpha} = [8, 000, 64, 000, 125, 000, 1,000, 000] \) and \( N = [2,376, 9,480, 14,760, 59,016] \), respectively. For \( \epsilon = 2 \) and all voxel sizes, the self-capacitance values computed by the VoxCap and FastCap simulators are compared with those obtained by the analytical formula, which reads as

\[
C = 4\pi \varepsilon \epsilon_0 (r_2 - r_1) / ((r_2 - r_1) + (r_2 - r_1)),
\]

where \( r_1 \) and \( r_2 \) are the radii of PEC sphere and dielectric shell, respectively; the relative difference between results \( \text{err} \) is plotted [Fig. 3(a)]. Apparently, while \( \text{err} \) decreases with increasing \( 1/\Delta r \), the accuracy achieved by both VoxCap and FastCap simulators is nearly the same. Their accuracy stagnates at the same level due
to staircase approximation to the spherical shape, which clearly appears in the normalized charge distributions plots for the structure discretized with \( \Delta v = [0.025, 0.01] \) m [Fig. 3(b)]. For the simulations of the structures discretized with \( \Delta v = [0.05, 0.025, 0.02, 0.01] \) m , the proposed VoxCap and FastCap simulators required CPU time of 

\[
1.54, 10.30, 11.75, 155.52 \text{ s} \quad \text{and} \quad 0.48, 2.02, 3.51, 14.26 \text{ s}
\]

and the memory of 

\[
8, 52, 97, 681 \text{ MB} \quad \text{and} \quad 135, 612, 992, 3009 \text{ MB},
\]

respectively. Note that the Tucker enhancement reduces the memory requirement from 2,440 MB to 681 MB (more than a factor of three and a half) for the analysis of the structure discretized with \( \Delta v = 0.01 \) m. It is expected that the VoxCap is much more memory efficient compared to FastCap while the FastCap is faster than VoxCap for this validation example with well-separated panels and high \( N_x / N \) ratio. It is shown below in the examples with densely-packed interconnects and low \( N_x / N \) ratios that the VoxCap is indeed much faster than FastCap for practical scenarios.

Next, \( \varepsilon_r \) is swept from 2 to \( 2 \times 10^2 \) with one-decade increment at each simulation of the structure discretized by \( \Delta v = 0.05 \) m [Fig. 3(c)]. Clearly, the proposed VoxCap produces accurate results for all \( \varepsilon_r \) values, while FastCap yields inaccurate results with increasing permittivity, as indicated in [31]. Finally, the effectiveness of the proposed preconditioner is examined for the structure discretized by \( \Delta v = 0.01 \) m and \( \varepsilon_r \) set to 2. For this case, the proposed VoxCap simulator iteratively solves (4) without using a preconditioner and with using the proposed block-diagonal-diagonal preconditioner, a diagonal preconditioner, and block-diagonal preconditioner. The blocks in proposed and block-diagonal preconditioners are formed by setting \( N_{x, y, z} = N_x = N_y = N_z = 10 \). For all these cases, RRE at each iteration is plotted [Fig. 3(d)]. The number of iterations required to reach \( 10^{-8} \) is 22, 27, 41 and 142 when the proposed preconditioner, the block diagonal preconditioner, the diagonal preconditioner, and no preconditioner are applied, respectively. Needless to say, the proposed preconditioner outperforms all other preconditioners and yields the fastest convergence. Furthermore, it requires 17.04 MB memory, a quarter of 70.26 MB memory requirement of the conventional block-diagonal preconditioner.

B. The PEC Cube

The proposed VoxCap simulator and FastCap simulator (with 4th order multipole expansion) are used to obtain the self-capacitance of a PEC cube with an edge length of 1 mm [Fig. 4(a)]. The cube is discretized by voxels of size \( \Delta v = [0.05, 0.025, 0.02, 0.01] \) mm , which gives rise to \( N_x = [8, 000, 64, 000, 125, 000, 1,000,000] \) and \( N = [2,400, 9,600, 15,000, 60,000] \), respectively. The self-capacitance computed by the VoxCap and FastCap for each voxel size is shown in [Fig. 4(a)]. Clearly, the capacitance obtained by VoxCap is more accurate and the result obtained for coarse discretization rapidly converges to that obtained for dense discretization. The proposed VoxCap and FastCap simulators required CPU time of 

\[
[0.71, 5.39, 6.42, 8.41] \text{ s} \quad \text{and} \quad [0.31, 1.14, 2.38, 8.56] \text{ s}
\]

and memory of 

\[
[8, 52, 97, 692] \text{ MB} \quad \text{and} \quad [33, 171, 259, 1026] \text{ MB},
\]

respectively.
respectively. Note that the Tucker enhancement reduces the memory footprint of the simulator from 1,321 MB to 692 MB (nearly a factor of two) for the analysis of the structure discretized with $\Delta v = 0.01$ m. Normalized charge distributions are plotted for the structure discretized with $\Delta v = [0.025, 0.01]$ mm [Fig. 4(b)].

Finally, the effectiveness of the proposed preconditioner is examined for the structure discretized by $\Delta v = 0.01$ m. For this case, the proposed VoxCap simulator iteratively solved (4) without using a preconditioner and with using the proposed preconditioner with only block-diagonal part (and without diagonal part since no dielectric exist in the scenario). The blocks in the preconditioner are formed using $N_x = N_y = N_z = 10$. For both cases, RRE at each iteration is plotted [Fig. 4(c)]. The number of iterations required to reach to $10^{-8}$ is 26 and 45 when the proposed preconditioner and no preconditioner are applied, respectively. For this example, the proposed preconditioner requires 68.7 MB memory, which is one-tenth of overall memory requirement 692 MB.

C. Numerical Tests on Tucker Enhancement

In this part, the memory saving achieved by and computational overhead introduced by Tucker decomposition are investigated while compressing and restoring the circulant tensors. In addition, the computational saving achieved by obtaining the Toeplitz tensors from their compressed representations is demonstrated. To this end, the memory saving is quantified via compression ratio (CR), which is the ratio of memory requirement of original tensors to the memory requirement of the compressed tensor. Furthermore, the computational overhead (CO) is quantified by taking the ratio of the time for restoring the tensor to the time for performing one convolution with that tensor.

1) A dielectric coated PEC plate: First, a dielectric coated PEC plate with varying width and length is considered to test the performance of Tucker compression/decompression for a 2D-like structure [Fig. 5 (a)]. The structure fully enclosed by the computational domain has the length and width varying from 100 $\mu$m to 1500 $\mu$m while $\Delta v = 1$ $\mu$m. For the structure with varying dimensions, Tucker decomposition is used to compress the circulant tensors; the CR achieved by and CO imposed by the Tucker decomposition are plotted in Figs. 5(a) and (b). Clearly, CR increases with increasing tolerance and the structure size (or number of voxels $N_t$). Tucker enhancement achieves more than 700x reduction (for $tol = 10^{-4}$ ) in the memory of circulant tensors for the largest structure. Moreover, CO decreases with increasing computational domain size and reaches to 0.05 for the largest structure size, which shows that the computational penalty associated with the tensor restoration operation is negligible. This negligible penalty is due to the fact the multilinear ranks of the compressed tensors remain nearly constant with increasing computational domain size. Fig. 5(c) demonstrates the change of the maximum multilinear rank of $\tilde{T}$ (as an example) with increasing $N_t$ for different tol values. Clearly, the maximum rank is a nearly constant function of $N_t$ and changes between 10 and 30. Fig. 5(d) shows the memory requirement of the original tensors as well as the compressed tensors with increasing structure size. Needless to say, the memory of original tensors scales with $O(t^3)$ while the memory of compressed tensors scales with $O(N_t^{0.44} \log(N_t))$. 

![Fig. 4. PEC cube example: (a) The self-capacitance obtained by VoxCap and FastCap with decreasing voxel size. (b) The normalized charge distribution on the structure when $\Delta v = 0.025$ mm (left) and $\Delta v = 0.01$ mm (right). (c) The RRE history of the LSE’s iterative solution when the proposed preconditioner and no preconditioner are applied.](image)
2) A dielectric coated cube: Next, a dielectric coated PEC cube with varying edge length is considered for testing the performance of Tucker compression/decompression for a 3D structure [Fig. 6(a)]. The cube fully enclosed by the computational domain has the edge length changed from 63 μm to 400 μm while Δv = 1 μm. For the structure with varying edge length, the circulant tensors are compressed by Tucker decompositions. The CR achieved by and CO introduced by Tucker compression and decompression are plotted in Figs. 6(a) and (b), respectively. Again, the CR increases with increasing tolerance and structure size (or number of voxels \( N_f \)). Tucker enhancement achieves more than 10000x (four orders of magnitude) reduction (for \( tol = 10^{-4} \)) in the memory of circulant tensors for the largest structure. Compared to dielectric coated PEC plate case, this dramatic reduction is expected as the tensor methods yield much better compression for the tensors with many elements along all three dimensions compared to the tensors with many elements along two dimensions and less elements in the remaining dimension, as in dielectric coated PEC plate case. Moreover, CO decreases with increasing structure size and reaches to 0.154 for the largest structure size for different \( tol \) values. This again shows that the computational penalty associated with the tensor restoration operation is negligible. Fig. 6(c) shows the change of the maximum multilinear rank of \( \mathbf{T}^{\perp} \) with increasing \( N_f \) for different \( tol \) values. Clearly, the maximum rank negligibly increases in the range from 10 to 20. Fig. 6(d) demonstrates the memory requirement of the original tensors as well as the compressed tensors with increasing structure size. While the memory of original tensors scales with \( O(N_f) \), the memory of compressed tensors scales with \( O(N_f^{10.26} \log(N_f)) \), which is better than \( O(N_f^{0.44} \log(N_f)) \) obtained for the dielectric-coated PEC plate.

3) Performance on Toeplitz Tensor: Next, the computational time saving achieved by obtaining Toeplitz tensors from their
Tucker-compressed versions is quantified. To this end, the dielectric coated cube in the previous analysis is considered. Its edge length is changed from 100 μm to 400 μm with increment of 100 μm while Δν = 1 μm. For the analysis of cube with different edge lengths, the memory requirement of the original Toeplitz tensors and Tucker-compressed Toeplitz tensors are tabulated in Table I. Furthermore, the CPU time required to generate original Toeplitz tensor and the CPU time required to obtain the Toeplitz tensor from Tucker-compressed Toeplitz tensors are provided. Apparently, the compressed tensors stored on hard disk require a few MBs memory for tol = 10⁻⁸ while the original ones require around 1 GB memory for the largest structure. While the CPU time to obtain the Toeplitz tensors is around 1.3 hours for the largest structure, the total CPU time to obtain the Toeplitz tensors from compressed tensors (including the CPU time for reading from harddisk and restoration from the compressed tensors) is 1.04 second for the same structure. By obtaining the Toeplitz tensors from Tucker compressed ones, 4655x speed-up is achieved for the largest structure.

D. Parallel Interconnects

In this practical example, a ten by ten parallel interconnect array embedded in a dielectric substrate (ε<sub>r</sub> = 10) with 1 mm spacing from the surfaces of the substrate is considered [Fig. 7(a)]. The width, length, and height of each interconnect are 5, 18, and 5 mm, respectively, while the center-to-center distance between interconnects is 6 mm. The discretization of the structure with \( \Delta v = 1 \) mm yields \( N_x = 74,420 \) and \( N = 53,322 \) (note that \( N_x/N = 1.3957 \)). The VoxCap with \( N_x = N_y = N_z = 5 \) and FastCap with 2<sup>nd</sup>, 4<sup>th</sup>, and 6<sup>th</sup> order multipole expansions are used to obtain the capacitance matrix for the structure. Figs. 7(a)-(c) compare the values in the first column of the capacitance matrix obtained by the VoxCap and the FastCap with (a) 2<sup>nd</sup> order and (b) 4<sup>th</sup> order multipole expansions, as well as (c) 6<sup>th</sup> order multipole expansions and normalized charge distribution on the structure (for the illustration purposes, the panels on dielectric substrate with x-coordinates larger than 0.0195 m were removed).

### TABLE I

| Edge length of cube (μm) | Memory of original Toeplitz tensors (MB) | Memory for compressed tensors (MB) | CPU time to generate original Toeplitz tensors (s) | CPU time to obtain Toeplitz tensors from compressed tensors (s) |
|--------------------------|----------------------------------------|-----------------------------------|-----------------------------------------------|-------------------------------------------------|
| 100                      | 15.72                                  | 1.57                              | 85.27                                        | 0.21                                            |
| 200                      | 123.91                                 | 2.76                              | 616.39                                       | 0.58                                            |
| 300                      | 416.12                                 | 3.91                              | 1858.59                                      | 0.822                                          |
| 400                      | 983.91                                 | 5.10                              | 4841.59                                      | 1.04                                            |

E. Parallel Meander Lines

Next, the parallel meander line structure is considered to check the accuracy and capabilities of the proposed VoxCap simulator [Fig. 8]. The structure is formed by the interconnects with the width \( w_s \), length \( l_b \), height \( h_b \), and spacing \( d \). There exist \( n \) number of interconnects in each of \( n \) number of layers. For the first analysis, after setting \( w_s = h_b = 0.5 \) mm.
The structure is discretized by $\Delta v = 0.1 \text{ mm}$, which yields $N_v = 1,416,100$ and $N = 808,600$ (note that $N_v / N = 1.7513$). For this case, the values in the first column of the capacitance matrix obtained by VoxCap with $N_{vx} = N_{vy} = N_{vz} = 10$ and FastCap with $2^{nd}$, $4^{th}$, and $6^{th}$ order multipole expansions are compared in Figs. 9(a)-(c). Furthermore, Fig. 9(c) also shows the normalized charge distribution on the structure obtained by VoxCap. The results obtained by FastCap with $6^{th}$ order of multipole expansion perfectly match with the results obtained by VoxCap. The average relative difference between results obtained by VoxCap and FastCap with $2^{nd}$, $4^{th}$, and $6^{th}$ order multipole expansions are 0.064, 0.008, and 0.002, respectively.

The memory and CPU time requirements of both simulators are tabulated in Table III. For nearly the same level of accuracy, the VoxCap required 30x less memory and 5x less CPU time compared to the FastCap with $6^{th}$ order multipole expansion.

Finally, a very large-scale parallel meander line structure is formed by setting $w_b = h_b = 0.5 \text{ mm}$, $d = 0.1 \text{ mm}$, $l_b = 50 \text{ mm}$, and $n = 100$. The discretization of this structure by $\Delta v = 0.1 \text{ mm}$ yields $N_v = 179,400,500$ and $N = 100,203,000$ ($N_v / N = 1.79$). For this example, the detailed breakdown of the memory and CPU usage of the VoxCap simulator is provided in Table IV. It is apparent in Table IV that the Tucker decomposition reduces the memory requirement of the circulant tensors from 132 GB to 6.8627 MB ($\text{for } tol = 10^{-4}$); it achieves a CR more than 19,000 while imposing a CO around 0.01. Furthermore, by reading the Tucker compressed Toeplitz tensors and restoring them, the VoxCap reduces the time for obtaining circulant tensors from 3832.63 seconds to 83.1 seconds; it achieves 46x speed-up. When the number of voxels in each small box for the preconditioner is increased from $N_{vx} = N_{vy} = N_{vz} = 10$ to $N_{vx} = N_{vy} = N_{vz} = 20$, the memory requirement of the preconditioner is increased from 320 MB to 19.5 GB, but the solution time is reduced nearly by a factor of 1.8 (from 47,620 secs to 26,773 secs) (Table IV). Fig. 9(d) shows the values in the one column of the capacitance matrix obtained by the VoxCap simulator. Note that the FastCap cannot be executed for this large-scale example due to its high memory cost. Fig. 9(d) also presents the normalized charge distribution on the structure by zooming into the opposite corners of the structure.
first column of the capacitance matrix obtained by the VoxCap and the normalized charge distribution on the structure and on its left lower and right upper corners.

| TABLE IV | THE DETAILED BREAKDOWN OF THE CPU TIME AND MEMORY USAGE FOR THE PARALLEL MEANDER LINE. UNITS FOR MEMORY AND CPU TIME ARE MB AND S. |
|-----------------|---------------------------------------------------------------|
| CPU time for pre-processing | 1365.8 |
| Memory of original $\mathcal{P}^{\alpha \beta \gamma}$ | 132,099.6 |
| Memory of compressed $\mathcal{P}^{\alpha \beta \gamma}$ | 6.8627 |
| CPU time for reading compressed Toeplitz tensors from hard disk | 0.10129 |
| CPU time for restoring compressedToeplitz tensors and embedding circulant tensors | 83 |
| CPU time for filling Toeplitz tensors and embedding circulant tensors | 3832.63 |
| CPU time for compressing and fast Fourier transforming the circulant tensors | 1.5578 |
| CPU time / memory for the preconditioner ( $N_\alpha = N_\gamma = N_\gamma = 10$ ) | 195.33 / 320.27 |
| CPU time / memory for the preconditioner ( $N_\alpha = N_\gamma = N_\gamma = 20$ ) | 245.88 / 19,500.1 |
| Number of iterations / CPU time for the solution when bottom conductor is excited (for $N_\alpha = N_\gamma = N_\gamma = 10$ ) | 242 / 47620.00 |
| Number of iterations / CPU time for the solution when bottom conductor is excited (for $N_\alpha = N_\gamma = N_\gamma = 20$ ) | 157 / 26773.02 |

IV. CONCLUSION

In this paper, VoxCap, a Tucker-enhanced and FFT-accelerated SIE simulator for electrostatic analysis and capacitance extraction of voxelized structures, was introduced. The VoxCap solves SIEs after discretizing the charge densities on panels by piecewise constant basis functions, applying Galerkin testing, and obtaining an LSE. The proposed VoxCap simulator uses FFTs to accelerate the MVMs during the iterative solution of LSE. Furthermore, it makes use of a highly effective and memory-efficient block-diagonal-diagonal preconditioner to reduce the number of iterations. It exploits Tucker decompositions to reduce its setup time and memory footprint. The proposed VoxCap simulator can solve problems with hundreds of million unknowns on a desktop computer. For many practical scenarios comprising densely packed interconnects, it is much faster and memory efficient compared to the FastCap. For example, for a parallel bus scenario considered in the numerical example section, the proposed VoxCap is more than 2.5x faster than FastCap while it requires more than 15x less memory compared to FastCap for the same accuracy.

APPENDIX A

ANALYTICAL EXPRESSION FOR THE RESULT OF INTEGRAL IN (6)

The analytical expression for the result of the integral in (5) is given in Appendix C of [25]. However, no analytical expression for the result of the integral in (6) was found in the literature. To this end, we derived the analytical expression of the result of the integral in (6) by computing the derivative of the analytical expressions in [25] and provide here. For the parallel panel interactions, the result of the integral in (6), $I$, is obtained as

$$I = \sum_{i=1}^{m} \sum_{n=1}^{N_{\alpha}} (-1)^{i+m} \left[ 0.5 a_i z \left( b_{n_{\alpha}} - 2 \right)^{-1} \right] \left( a_i + r_{n_{\alpha}} \right) r_{n_{\alpha}} + \epsilon 
- a_i z \log \left( a_i + r_{n_{\alpha}} + \epsilon \right) + \frac{0.5 b_{n_{\alpha}}^2 \left( a_i^2 - z^2 \right)}{\left( b_{n_{\alpha}} + r_{n_{\alpha}} \right)^2 + \epsilon} 
- b_{n_{\alpha}}^2 \log \left( b_{n_{\alpha}} + r_{n_{\alpha}} + \epsilon \right) + \frac{2 \pi r_{n_{\alpha}}^2}{3} - z \left( a_i^2 + b_{n_{\alpha}}^2 - 2 z^2 \right) \right] \quad (16)$$

where $a_i = x_{i2} - x_{i1}$, $a_2 = x_{i2} - x_{i1}$, $a_3 = x_{i2} - x_{i1}$, $a_4 = x_{i2} - x_{i1}$, $b_1 = y_{i2} - y_{i1}$, $b_2 = y_{i2} - y_{i1}$, $b_3 = y_{i2} - y_{i1}$, $b_4 = y_{i2} - y_{i1}$, $z = z_i - z_i + \epsilon$. $r_{n_{\alpha}} = \sqrt{a_i^2 + b_{n_{\alpha}}^2 + z^2}$, and $\epsilon = 10^{-37}$. The geometrical quantities in these expressions are given in Fig. A(a). For the orthogonal interactions, the result of the integral in (6), $I$, is obtained as

$$I = \sum_{i=1}^{m} \sum_{n=1}^{N_{\alpha}} (-1)^{i+m} \left[ \frac{b_{n_{\alpha}}}{b_{n_{\alpha}} r_{n_{\alpha}}} \left( \frac{a_i^2 - b_{n_{\alpha}}^2}{r_{n_{\alpha}}^2} \right) + \frac{a_i b_n z \left( a_i b_n + a_i b_{n_{\alpha}} \right)}{r_{n_{\alpha}}^2 + z^2} \right] \right) \frac{\pi}{6 r_{n_{\alpha}}^2} \left( b_{n_{\alpha}} + r_{n_{\alpha}} + \epsilon \right) + \frac{a_i b_n e^{-r_{n_{\alpha}}^2}}{r_{n_{\alpha}} (a_i^2 + c_{i_{\alpha}}^2)} + \frac{a_i b_n e^{-r_{n_{\alpha}}^2}}{r_{n_{\alpha}} (a_i^2 + c_{i_{\alpha}}^2)} - 2 \arctan \left( \frac{a_i b_n}{c_{i_{\alpha}}} + \epsilon \right) \right] \quad (17)$$

where $a_i = x_{i2} - x_{i1}$, $a_2 = x_{i2} - x_{i1}$, $a_3 = x_{i2} - x_{i1}$, $a_4 = x_{i2} - x_{i1}$, $b_1 = y_{i2} - y_{i1}$, $b_2 = y_{i2} - y_{i1}$, $c_1 = z_i - z_i + \epsilon$. $r_{n_{\alpha}} = \sqrt{a_i^2 + b_{n_{\alpha}}^2 + c^2}$, and $\epsilon = 10^{-37}$. The geometrical quantities in these expressions are provided in Fig. A(b).
and are obtained by, respectively. To this end, the procedure explained in the Appendix B of [17] is followed. The signs of the Toeplitz blocks used to construct the blocks of circulant tensors are assigned as in Table VII. Note that this table corresponds to Table 5 of [17] and the blocks in circulant tensors are labeled by L, M, N, LM, LN, MN, as in [17].

The block circulant tensors \( \mathbf{P}^{\alpha,\beta} \) and \( \mathbf{E}^{\alpha,\beta} \) are obtained by properly embedding the block Toeplitz tensors \( \mathbf{A}^{\alpha,\beta} \) and \( \mathbf{B}^{\alpha,\beta} \), respectively. To reduce the number of FFT and IFFT operations, as mentioned above. The locations of tensor entries for padding zeros are provided in Table IX.

The embedding process generates the block circulant tensors \( \mathbf{P}^{\alpha,\beta} \) and \( \mathbf{E}^{\alpha,\beta} \) with dimensions given in Table VIII. These dimensions are enlarged to \( 2(N_i+1)\times 2(N_i+1) \) by proper zero-padding to reduce the number of FFT and IFFT operations, as mentioned above. The locations of tensor entries for padding zeros are provided in Table IX.
Algorithm 2 Procedure for generating $A^{α,β}$ and $B^{α,β}$.

Preprocessing: For given $(α, β)$ pair and $Δν$. To this end, consider the parallel panel configuration demonstrated in Fig. A(a). For this configuration, the integral in (5) is written as

$$I = \frac{1}{4\pi_0} \int \int \int K_1 d\nu' d\nu d\nu,$$  \hspace{1cm} (18)

where

$$K_1 = \frac{1}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}}.$$  \hspace{1cm} (19)

$z = z_1$ and $z' = z_2$. The integrals on primed coordinates are evaluated on the observer panel (top panel in Fig. A(a)) for the basis function while those on the non-primed coordinates are evaluated on the source panel (bottom panel in Fig. A(a)) for testing function. In the voxelized setting, the source and observer panels sit on grid points with indices $(m_1, m_2, m_3)$ and $(m_1, m_2, m_3)$. To this end, first the bounds are changed as $x_2 = m_1Δν$, $x_3 = (m_1 + 1)Δν$, $y_2 = m_1Δν$, $y_3 = (m_1 + 1)Δν$, and $z_3 = cΔν$, and $z'_3 = cΔν$ in (18), which yields

$$I = (Δν^3) \frac{1}{4\pi_0} \int \int \int K_2 d\nu' d\nu d\nu,$$  \hspace{1cm} (20)

where

$$K_2 = \frac{1}{\sqrt{(a-a')^2 + (b-b')^2 + (c-c')^2}}.$$  \hspace{1cm} (21)

Apparently, the integral of (20) is independent from voxel size and thereby scaling factor is $Δν^3$ for the parallel panel interactions. Similarly, the scaling factor is obtained as $Δν^3$ for the orthogonal panel interactions by applying the same procedure. For the same parallel panel configuration, the integral in (6) is written as

$$I = \frac{1}{4\pi_0} \int \int \int K_3 d\nu' d\nu d\nu,$$  \hspace{1cm} (22)

where

$$K_3 = \frac{1}{\sqrt{(a-a')^2 + (b-b')^2 + (c-c')^2}}.$$  \hspace{1cm} (23)

After changing the bounds of integrals and applying the change of variables and constants as described above, the integral in (22) is obtained as

$$I = (Δν^3) \frac{1}{4\pi_0} \int \int \int (z-z') K_3 d\nu' d\nu d\nu.$$  \hspace{1cm} (24)

Needless to say, the scaling factor is $Δν^3$ for parallel panel interactions. The same scaling factor is obtained for the orthogonal panel interactions.

**Algorithm 2**

Preprocessing: For given $(α, β)$ pair and $Δν$. To this end, consider the parallel panel configuration demonstrated in Fig. A(a). For this configuration, the integral in (5) is written as

$$I = \frac{1}{4\pi_0} \int \int \int K_1 d\nu' d\nu d\nu,$$  \hspace{1cm} (18)

where

$$K_1 = \frac{1}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}}.$$  \hspace{1cm} (19)

$z = z_1$ and $z' = z_2$. The integrals on primed coordinates are evaluated on the observer panel (top panel in Fig. A(a)) for the basis function while those on the non-primed coordinates are evaluated on the source panel (bottom panel in Fig. A(a)) for testing function. In the voxelized setting, the source and observer panels sit on grid points with indices $(m_1, m_2, m_3)$ and $(m_1, m_2, m_3)$. To this end, first the bounds are changed as $x_2 = m_1Δν$, $x_3 = (m_1 + 1)Δν$, $y_2 = m_1Δν$, $y_3 = (m_1 + 1)Δν$, and $z_3 = cΔν$, and $z'_3 = cΔν$ in (18), which yields

$$I = (Δν^3) \frac{1}{4\pi_0} \int \int \int K_2 d\nu' d\nu d\nu,$$  \hspace{1cm} (20)

where

$$K_2 = \frac{1}{\sqrt{(a-a')^2 + (b-b')^2 + (c-c')^2}}.$$  \hspace{1cm} (21)

Apparently, the integral of (20) is independent from voxel size and thereby scaling factor is $Δν^3$ for the parallel panel interactions. Similarly, the scaling factor is obtained as $Δν^3$ for the orthogonal panel interactions by applying the same procedure. For the same parallel panel configuration, the integral in (6) is written as

$$I = \frac{1}{4\pi_0} \int \int \int K_3 d\nu' d\nu d\nu,$$  \hspace{1cm} (22)

where

$$K_3 = \frac{1}{\sqrt{(a-a')^2 + (b-b')^2 + (c-c')^2}}.$$  \hspace{1cm} (23)

After changing the bounds of integrals and applying the change of variables and constants as described above, the integral in (22) is obtained as

$$I = (Δν^3) \frac{1}{4\pi_0} \int \int \int (z-z') K_3 d\nu' d\nu d\nu.$$  \hspace{1cm} (24)

Needless to say, the scaling factor is $Δν^3$ for parallel panel interactions. The same scaling factor is obtained for the orthogonal panel interactions.
REFERENCES

[1] A. C. Yucel, I. P. Georgakas, A. G. Polimeridis, H. Bagei, and J. K. White, "VoxHenry: FET-accelerated inductance extraction for voxelized geometries," IEEE Trans. Microw. Theory Techn., vol. 66, no. 4, pp. 1723–1735, Apr. 2018.

[2] M. Naghd and I. Wolff, "A three-dimensional finite-difference calculation of equivalent capacitances of coplanar waveguide discontinuities," presented at the IEEE International Digest on Microwave Symposium, Dallas, TX, USA, May, 1990.

[3] A. H. Zemanian, "A finite-difference procedure for the exterior problem inherent in capacitance computations for VLSI interconnections," IEEE Trans. Electron Devices, vol. 35, no. 7, pp. 985-992, July 1988.

[4] Z. Zhu and W. Hong, "A generalization algorithm for the capacitance extraction of 3D VLSI interconnects," IEEE Trans. Microw. Theory Technol., vol. 47, no. 10, pp. 2027 - 2030, Oct. 1999.

[5] G. Chen, H. Zhu, T. Cui, Z. Chen, X. Zeng, and W. Cai, "ParAFEMCap: A parallel adaptive finite-element method for 3-D VLSI interconnect capacitance extraction," IEEE Trans. Microw. Theory Techn., vol. 60, no. 2, pp. 218–231, Feb. 2012.

[6] R. Sabelka and S. Selberherr, "A finite element simulator for three-dimensional analysis of interconnect structures," Microelectron.J., vol. 32, no. 2, pp. 163-171, Feb. 2001.

[7] W. Proskurowski and O. Widlund, "A Finite Element-Capacitance Matrix Method for the Neumann Problem for Laplace’s Equation," SIAM J. Sci. and Stat. Comput., vol. 1, no. 4, pp. 410–425, July 2006.

[8] A. G. Polimeridis, J. F. Villena, L. Daniel, and J. K. White, "FastCap: A multipole accelerated 3-D capacitance extraction program," IEEE Trans. Comput-Aided Design, vol. 11, no. 11, pp. 1447-1459, Nov. 1991.

[9] W. Shi, J. Liu, N. Kakani, and T. Yu, "A fast hierarchical algorithm for three-dimensional capacitance extraction," IEEE Trans. Comput-Aided Design Integ. Circuits Syst., vol. 21, no. 3, pp. 330–336, Mar. 2002.

[10] D. Gope and V. Jandhyala, "PILOT: a fast algorithm for enhanced 3D parasitic capacitance extraction efficiency," Microwave Opt. Tech. Lett., vol. 41, no. 3, pp. 169-173, May 2004.

[11] D. Gope and V. Jandhyala, "Oct-tree-based multilevel low-rank decomposition algorithm for rapid 3-D parasitic extraction," IEEE Trans. Comput. Aid Design Integ. Circuits Syst., vol. 23, no. 11, pp. 1575-1580, Nov. 2004.

[12] K. Nabors and J. White, "FastCap: A multipole accelerated 3-D capacitance extraction program," IEEE Trans. Computer-Aided Design, vol. 11, no. 11, pp. 1447-1459, Nov. 1991.

[13] J. R. Phillips and J. K. White, "A precorrected-FFT method for electrostatic analysis of complicated 3-D structures," IEEE Trans. Comput-Aided Design, vol. 16, no. 10, pp. 1059-1072, Oct. 1997.

[14] A. G. Polimeridis, J. F. Villena, L. Daniel, and J. K. White, "Stable FET-JVIE solvers for fast analysis of highly inhomogeneous dielectric objects," J. Comp. Phys., vol. 269, pp. 280-296, 2014.

[15] 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, May 1989.

[16] H. Gan and W. C. Chew, "A discrete BCG-FET algorithm for solving 3D inhomogeneous scatterer problems," J. Electromagn. Waves Appl., vol. 9, pp. 1339–1357, Apr. 1995.

[17] A. C. Yucel, W. Sheng, C. Zhou, Y. Liu, H. Bagci, and E. Michielssen, "An FMM-FMT 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.

[18] M. F. Catedra, R. F. Torres, J. Basterrech, and E. Gago, The CG-FET Method: Application of Signal Processing Techniques to Electromagnetics. Norwood, MA: Artech House, 1995.

[19] M. Wang, C. Qian, and A. C. Yucel, "Tucker-enhanced VoxCap simulator for electrostatic analysis of voxelized structures," in Proc. IEEE MIT-S Int. Conf. on Numer. EM and Multiphysics Modeling and Opt., Boston 2019.

[20] K. Nabors and J. White, "Multipole-accelerated capacitance extraction algorithms for 3-D structures with multiple dielectrics," IEEE Trans. Circuits Syst., vol. 39, no. 11, pp. 946-954, Nov. 1992.

[21] K. S. Nabors, "Efficient Three-Dimensional Capacitance Calculation," Ph.D. Massachusetts Institute of Technology, Cambridge, MA, USA, 1993.

[22] A. F. Ruehli, G. Antonini, and L. Jiang, Circuit Oriented Electromagnetic Modeling Using the PEEC Techniques. John Wiley & Sons, 2017.

[23] A. C. Yucel, "Uncertainty quantification for electromagnetic analysis via efficient collocation methods," Ph.D. dissertation, Univ. Michigan, Ann Arbor, MI, USA, 2013.

[24] L. D. Lathauer, B. D. Moor, and J. Vandewalle, "A multilinear singular value decomposition," SIAM J. Matrix Anal. Appl., vol. 21, no. 4, pp. 1253-1278, 2000.

[25] A. C. Yucel, L. J. Gomez, and E. Michielssen, "Compression of translation operator tensors in FMM-FET accelerated SIE solvers via Tucker decomposition," IEEE Antennas Wireless Propag. Lett., vol. 16, pp. 2667-2670, 2017.

[26] C. Qian, Z. Chen, and A. C. Yucel, "Tensor decompositions for reducing the memory requirement of translation operator tensors in FMM-FET accelerated IE solvers," presented at the Proc Applied Computational EM Society (ACES) Symp., Miami, FL, USA, April 2019.

[27] T. Kolda and B. Bader, "Tensor decompositions and applications," SIAM Review, vol. 51, no. 3, pp. 455-500, Sep. 2009.

[28] Y. Massoud, J. Wang, and J. White, "Accurate inductance extraction with permeable materials using qualocation," presented at the Proceedings of the International Conference on Modeling and Simulation of Micromsystems, April 1999.

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