High-Order Accurate Integral Equation Based Mode Solver for Layered Nanophotonic Waveguides

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***Abstract* — We present a novel high-order boundary integral equation based mode solver for layered nanophotonic waveguides featuring corners and junctions. The proposed solver leverages an indirect single-trace formulation for composite dielectrics which leads to a Müller-like integral equation posed on the cross-section of the material interfaces, and a high-order Nyström discretization for domains with corners. A variety of numerical examples demonstrate the superior accuracy of the proposed methodology as compared to standard commercial finite element and finite difference based mode solvers.**

***Keywords* — mode solver, dielectric waveguides, nanophotonics, layered media, integral equations.**

I. Introduction

Waveguides are fundamental components of photonic integrated circuits (PICs) which are used to efficiently guide and propagate light between optical devices on a chip. A nanophotonic waveguide is typically composed of a dielectric core material sitting on top of a dielectric substrate (Fig. 1). Since PICs are often too large and complex to simulate in their entirety, the underlying optical building blocks are simulated and designed in isolation with their ports attached to semi-infinite incoming/input and outgoing/output nanophotonic waveguides. The characterization of waveguide modes is then needed to properly model the system.

Several numerical techniques exist for finding the modes of a given waveguide structure, and in fact multiple commercial mode solvers exist which leverage finite-difference (FD) and finite element (FE) methods. Unfortunately, these methods are typically only 1st or 2nd order accurate, and can lead to large and costly sparse eigenvalue problems. A highly accurate numerical mode-matching method is presented in [1]. However, this method is limited to waveguide cross-sections which only have perfectly horizontal or vertical material interfaces. A highly accurate but rather involved boundary integral equation (BIE) approach, that can be used to simulate arbitrary piecewise homogeneous dielectric waveguide cross-sections, is presented in [2]. Unlike the formulation in [2], which requires the evaluation of hypersingular integral operators that can be challenging and difficult to implement accurately, in this work we present a novel BIE-based mode solver based on a single-trace Müller-like (STM) formulation that can easily deal with composite waveguides featuring triple or multiple junctions. Our formulation only involves the calculation of weakly singular integrals which can be readily computed with high accuracy using simple quadrature rules that maintain their precision for structures with sharp corners and junctions. Furthermore, the proposed formulation is well-conditioned away from the sought mode frequencies, allowing the use of GMRES for the rapid evaluation of the suitable function used to solve for the modes.

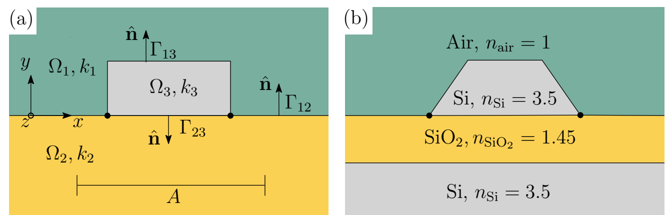

Fig. 1. (a) Cross-section of the waveguide structure considered in the model problem. (b) Trapezoidal-shape waveguide considered in section IV.

II. Model problem formulation

Our model problem consists of an optical waveguide placed on top of a layered dielectric plane (see Fig. 1a) which may consist of an arbitrary number of layers. The waveguide structure, which is assumed to occupy the cylinder $D_3 = \Omega_3 \times (-\infty, \infty)$ of cross section Ω_3 in the xy plane, has permittivity and permeability denoted by ϵ_3 and μ_3, respectively. Similarly, the upper $D_1 = \Omega_1 \times (-\infty, \infty)$ (resp. lower $D_2 = \Omega_2 \times (-\infty, \infty)$) domain has material constants ϵ_1 and μ_1 (resp. ϵ_2 and μ_2). Assuming the time dependence of the electromagnetic field is $\mathrm{e}^{-i\omega t}$ where ω is the angular frequency, our goal is to find non-trivial EM fields $(\mathbf{E}_j, \mathbf{H}_j)$ in D_j, $j = 1, 2, 3$, such that the (normalized) Maxwell's equations $\nabla \times \mathbf{E}_j - ik_j\mathbf{H}_j = \mathbf{0}$ and $\nabla \times \mathbf{H}_j + ik_j\mathbf{E}_j = \mathbf{0}$ in D_j, and the transmission conditions

$$\begin{aligned} \hat{\mathbf{n}} \times \left\{\sqrt{\mu_j}\mathbf{E}_j|_- - \sqrt{\mu_i}\mathbf{E}_i|_+\right\} &= \mathbf{0} \\ \hat{\mathbf{n}} \times \left\{\sqrt{\epsilon_j}\mathbf{H}_j|_- - \sqrt{\epsilon_i}\mathbf{H}_i|_+\right\} &= \mathbf{0} \quad \text{on} \quad S_{ij}, \end{aligned} \tag{1}$$

are satisfied, where $k_j = 2\pi/\lambda_j = \omega\sqrt{\epsilon_j\mu_j}$ is the wavenumber and $S_{ij} = \overline{D}_i \cap \overline{D}_j = \Gamma_{ij} \times (-\infty, \infty)$, $(i, j) = (1, 2)$, $(1, 3)$ and $(2, 3)$, are the material interfaces (see Fig. 1). Additionally, a suitable radiation condition is required so as to ensure the sought EM modes propagate away from the waveguide.

To enforce the conditions (1) and to take care of the junctions, we resort to a single-trace (indirect) BIE formulation [3], [4]. Letting $(\mathcal{H}_j\mathbf{A})(\mathbf{r}) = \nabla \times \int_S G_j(\mathbf{r}, \mathbf{r}')\mathbf{A}(\mathbf{r}')\,\mathrm{d}s'$ and $(\mathcal{E}_j\mathbf{A})(\mathbf{r}) := \frac{i}{k_j}\nabla \times (\mathcal{H}_j\mathbf{A})(\mathbf{r})$ for $\mathbf{r} \in \mathbb{R}^3 \setminus S$, with $G_j(\mathbf{r}, \mathbf{r}') = (4\pi|\mathbf{r} - \mathbf{r}'|)^{-1}\,\mathrm{e}^{ik_j|\mathbf{r}-\mathbf{r}'|}$ and $\mathbf{A}$

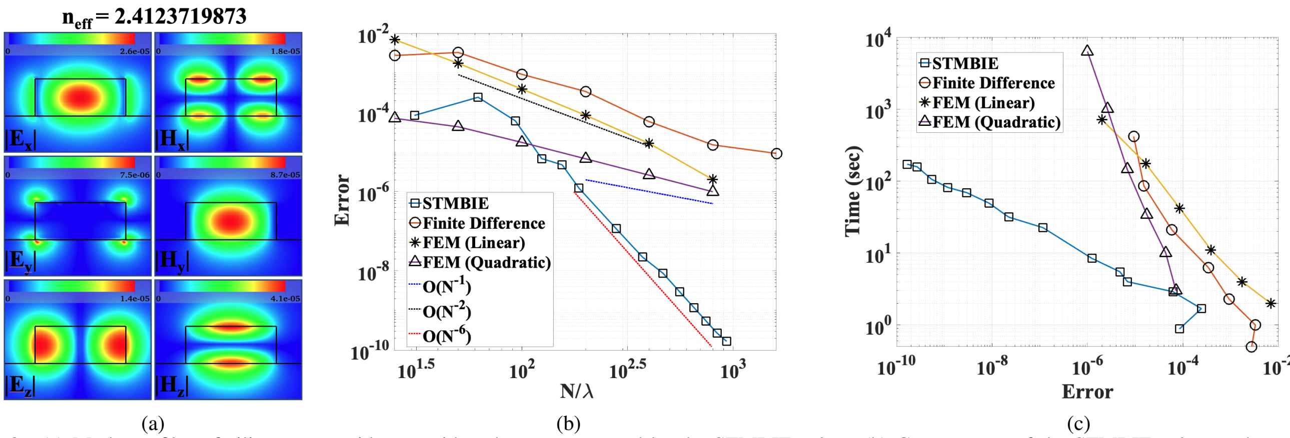

Fig. 2. (a) Mode profiles of silicon waveguide on oxide substrate computed by the STMBIE solver. (b) Convergence of the STMBIE solver and commercial FD and FEM solvers. A highly refined solution from the STMBIE solver is used as the reference solution. Dashed lines represent first-, second-, and sixth-order convergence for comparison. (c) Comparison of relative error vs. time required for the STMBIE and commercial solvers.

denoting a tangential vector field to the skeleton $S = \bigcup_{i,j} S_{ij}$ (i.e., the union of all material interfaces), the EM fields are sought in the form

$$\begin{aligned}\mathbf{E}_j(\mathbf{r}) &= \epsilon_j^{1/2}(\mathcal{E}_j\mathbf{J})(\mathbf{r}) - \mu_j^{1/2}(\mathcal{H}_j\mathbf{M})(\mathbf{r})\\ \mathbf{H}_j(\mathbf{r}) &= \epsilon_j^{1/2}(\mathcal{H}_j\mathbf{J})(\mathbf{r}) + \mu_j^{1/2}(\mathcal{E}_j\mathbf{M})(\mathbf{r})\end{aligned} \tag{2}$$

in terms of unknown surface currents $\mathbf{J}$ and $\mathbf{M}$ that are to be determined by enforcing the transmission conditions (1). Note that the off-surface operators $\mathcal{H}_j$ and $\mathcal{E}_j$ are defined by integrals over the entire skeleton S. Using the well-known jump relations: $\hat{\mathbf{n}}\times(\mathcal{H}_j\mathbf{A})|_\pm = \mathcal{K}_j\mathbf{A} \pm \frac{\mathbf{A}}{2}$ and $\hat{\mathbf{n}}\times(\mathcal{E}_j\mathbf{A})|_\pm = \mathcal{T}_j\mathbf{A}$, where

$$\begin{aligned}(\mathcal{K}_j\mathbf{A})(\mathbf{r}) &= \hat{\mathbf{n}}(\mathbf{r}) \times \nabla \times \int_S G_j(\mathbf{r},\mathbf{r}')\mathbf{A}(\mathbf{r}')\,\mathrm{d}s'\\ (\mathcal{T}_j\mathbf{A})(\mathbf{r}) &= \frac{i}{k_j}\hat{\mathbf{n}}(\mathbf{r}) \times \nabla \times \nabla \times \int_S G_j(\mathbf{r},\mathbf{r}')\mathbf{A}(\mathbf{r}')\,\mathrm{d}s'\end{aligned} \tag{3}$$

are the so-called MFIE and EFIE operators, respectively, we have

$$\begin{aligned}\sqrt{\mu_j}(\hat{\mathbf{n}}\times\mathbf{E}_j)|_\pm &= (k_j/\omega)\mathcal{T}_j\mathbf{J} - \mu_j\left\{\pm\mathbf{M}/2 + \mathcal{K}_j\mathbf{M}\right\}\\ \sqrt{\epsilon_j}(\hat{\mathbf{n}}\times\mathbf{H}_j)|_\pm &= (k_j/\omega)\mathcal{T}_j\mathbf{M} + \epsilon_j\left\{\pm\mathbf{J}/2 + \mathcal{K}_j\mathbf{J}\right\}.\end{aligned} \tag{4}$$

Imposing (1) by means of (4), we thus arrive at the following integral equation system:

$$\begin{aligned}\left\{(\mu_i+\mu_j)\,\mathbf{M} - 2(\mu_j\mathcal{K}_j - \mu_i\mathcal{K}_i)\mathbf{M} + \mathcal{T}_{ij}\mathbf{J}\right\}|_{S_{ij}} &= \mathbf{0}\\ \left\{(\epsilon_i+\epsilon_j)\,\mathbf{J} - 2(\epsilon_j\mathcal{K}_j - \epsilon_i\mathcal{K}_i)\mathbf{J} - \mathcal{T}_{ij}\mathbf{M}\right\}|_{S_{ij}} &= \mathbf{0},\end{aligned} \tag{5}$$

where $\mathcal{T}_{ij} = \frac{2}{\omega}(k_j\mathcal{T}_j - k_i\mathcal{T}_i)$, for $(i,j) \in \{(1,2),(1,3),(2,3)\}$. The sought modes are thus determined via (2) by the non-trivial solutions $\mathbf{M}$ and $\mathbf{J}$ of the homogeneous system (5). Note that, as in the case of the Müller formulation [5], all the integral operators in the 3D STMBIE (5) feature kernels with at most integrable $O(|\mathbf{r}|^{-1})$ singularities as $|\mathbf{r}| \to 0$.

III. Cross-section Integral Equation Formulation

Relying on the axial symmetry of the waveguide structure, we can recast (5) as a system of integral equations posed on the 2D skeleton cross section $\Gamma = \bigcup_{i,j}\Gamma_{ij}$. Indeed, since the sought EM fields $(\mathbf{E}_j, \mathbf{H}_j)$, $j = 1,2,3$, are completely determined by their z-components $E_{z,j}$ and $H_{z,j}$, which take the form $E_{z,j} = e_{z,j}(\boldsymbol{\rho})\,\mathrm{e}^{i\beta z}$ and $H_{z,j} = h_{z,j}(\boldsymbol{\rho})\,\mathrm{e}^{i\beta z}$ for some propagation constant β, it holds that the tangential surface currents can be expressed as $\mathbf{M}(\mathbf{r}) = \left\{M_\tau(\boldsymbol{\rho})\hat{\boldsymbol{\tau}}(\boldsymbol{\rho}) + M_z(\boldsymbol{\rho})\hat{\mathbf{k}}\right\}\mathrm{e}^{i\beta z}$ and $\mathbf{J}(\mathbf{r}) = \left\{J_\tau(\boldsymbol{\rho})\hat{\boldsymbol{\tau}}(\boldsymbol{\rho}) + J_z(\boldsymbol{\rho})\hat{\mathbf{k}}\right\}\mathrm{e}^{i\beta z}$, where $\mathbf{r} = (\boldsymbol{\rho}, z)$ and $\hat{\mathbf{n}} = \tau_2\hat{\mathbf{i}} - \tau_1\hat{\mathbf{j}}$ with $\hat{\boldsymbol{\tau}} = \tau_1\hat{\mathbf{i}} + \tau_2\hat{\mathbf{j}}$ denoting the unit tangent vector to Γ (see Fig. 1a). Therefore, replacing these expressions in (5) and employing the identity

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{i\beta z'}}{4\pi}\frac{\mathrm{e}^{ik_j|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}z' = \frac{i}{4}H_0^{(1)}\left(\kappa_j(\beta)|\boldsymbol{\rho}-\boldsymbol{\rho}'|\right)\mathrm{e}^{i\beta z}, \tag{6}$$

where $\kappa_j(\beta) = \sqrt{k_j^2 - \beta^2}$, (5) is recast as the following system of scalar 2D STMBIE:

$$\left\{\mathsf{E}_{ij}\boldsymbol{\varphi} + \mathsf{W}_{ij}(\beta)[\boldsymbol{\varphi}]\right\}|_{\Gamma_{ij}} = \mathbf{0}, \tag{7}$$

for $(i,j) \in \{(1,2),(1,3),(2,3)\}$, where $\mathsf{E}_{ij} = \mathrm{diag}(\mu_i + \mu_j, \mu_i + \mu_j, \epsilon_i + \epsilon_j, \epsilon_i + \epsilon_j)$ and $\boldsymbol{\varphi} = (M_\tau, M_z, J_\tau, J_z)$ is a vector density function defined on Γ. For the sake of conciseness, we do not make explicit the block entries of the rather involved integral operator $\mathsf{W}_{ij}(\beta)$ here (the block entries of W_{ij} are of the same form as in [6], which presents a similar Müller formulation for simple dielectric waveguides in free-space). Note that, in view of (6) and the fact that (5) is given in terms of operators with weakly-singular kernels, W_{ij} features kernels with $O(\log|\boldsymbol{\rho}|)$ singularities as $|\boldsymbol{\rho}| \to 0$.

IV. Mode Solver

In order to numerically find non-trivial solutions of (7), we leverage the exponential decay away from the core for both the waveguide modes and surface currents in $\boldsymbol{\varphi}$ [2]. Therefore, instead of attempting to solve (7) on the unbounded skeleton cross-section Γ, we solve it on a small portion Γ_A of Γ around Ω_3. The exponential decay of the currents $\boldsymbol{\varphi}$ gives rise to exponential decay of the errors in the approximation $\boldsymbol{\varphi} \approx \boldsymbol{\varphi}_A$ on Γ_A, as the truncation width A (see Fig. 1a) increases,

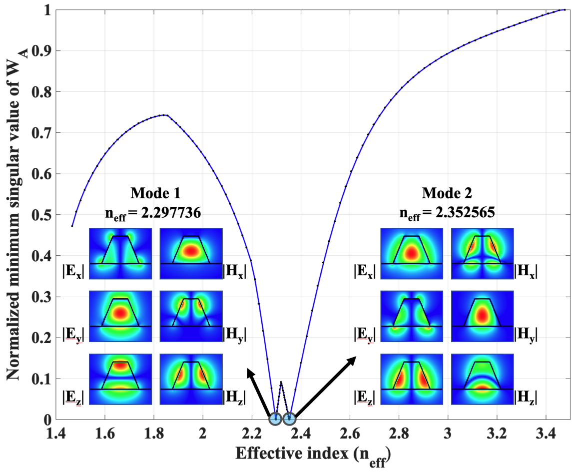

Fig. 3. Minimum singular value of $E + W_A$ vs. n_{eff} for a trapezoidal waveguide over a multi-layer SOI substrate. The two zeros indicate the existence of two propagating modes and their corresponding field profiles are superimposed. (The additional layers are not displayed in the inset figures for visualization purposes.)

where φ_A denotes the currents obtained by solving (7) on the truncated skeleton cross-section Γ_A. Given that W_{ij} features only weakly-singular kernels, the discretization of system (7) can be achieved using the high-order Nyström method for the 2D Helmholtz equation (including corners) presented in [7]. Finally, the waveguide modes are obtained by searching for values of β at which the matrix $E+W_A(\beta)$, resulting from the Nyström discretization of the integral equation on Γ_A, becomes singular. This is achieved by means of the strategy used in [6], which is to find the zeros of $f(\beta) = (\mathbf{y}^T(E+W_A(\beta))^{-1}\mathbf{x})^{-1}$ where $\mathbf{x}$ and $\mathbf{y}$ are two fixed random vectors independent of β. The function f is efficiently evaluated by means of the GMRES algorithm which is used to compute $(E+W_A(\beta))^{-1}\mathbf{x}$ iteratively. Evaluations of f can be accelerated by means of $\mathcal{H}$-matrix algorithms [8] or the fast multipole method [9].

V. Numerical Examples

We first compare the performance of our STMBIE approach against state-of-the-art FD and FE commercial software by solving for the fundamental mode of a 500×220nm silicon ($n_{\mathrm{Si}} = \sqrt{\epsilon_{\mathrm{Si}}} = 3.5$) waveguide on top of an infinitely thick oxide layer ($n_{\mathrm{SiO_2}} = \sqrt{\epsilon_{\mathrm{SiO_2}}} = 1.45$) with air above it (Fig. 1a). A free-space wavelength $\lambda = 1.55\mu$m is used corresponding to the common telecommunications band for both examples in this section. The same problem was also considered in [1] and [2], and the effective index $n_{\mathrm{eff}} = \frac{\lambda}{2\pi}\beta = 2.4123719873$ determined by our STMBIE method matches exactly with all 9 digits of their reported value. By using the representation formula (2) and the densities resulting from the solution of the 2D STMBIE (7), all six field components of the mode cross-section can be evaluated readily, as shown in Fig. 2a. In Fig. 2b we show the absolute error in the n_{eff} values computed using the proposed STMBIE and commercial FD and FE solvers for various discretizations. PMLs were used in the FD solver to simulate open boundaries and PEC boundary conditions were used in the FE solver. Both linear and quadratic FE basis functions were utilized in this comparison. The FD and linear FE methods exhibited 2nd-order convergence as expected; however, the quadratic FE method surprisingly only achieved 1st-order convergence. Our STMBIE, in turn, follows a 6th-order convergence slope, which is limited by the degree of the graded mesh utilized to cluster points near the corner singularities. Fig. 3c displays absolute wall time versus error required for each solver. As can be seen, the STMBIE approach requires less time than any of the other approaches to achieve a desired error, despite the fact that not much effort was placed into optimizing our prototype implementation. The timings were all measured on a server with dual Xeon Gold 6154 CPUs (36 cores). The STMBIE algorithm requires 10 times less memory than both FD and FE methods at the same mesh resolution.

Finally, in order to show that STMBIE can be applied to arbitrarily shaped waveguides (unlike, for example, the method presented in [1] which can only handle perfectly vertical and horizontal interfaces) as well as multi-layer substrates, we solve for all the propagation constants and mode profiles for the trapezoidal-shaped silicon waveguide depicted in Fig. 1b. The silicon guide is 350nm tall with a bottom width of 500nm and top width of 200nm. The oxide layer below is 1μm thick and sits on top of an infinite silicon substrate handle. The dielectric material parameters used are the same as in the first example. Fig. 3 plots the normalized minimum singular value of the STMBIE system matrix versus effective index, n_{eff}, together with the corresponding modal fields. Propagating modes correspond to zeros in this plot, and note that for this case, the STMBIE formulation is free from spurious solutions.

VI. Conclusion

A single-trace Müller boundary integral equation (STMBIE) formulation was presented which can numerically solve with high-order accuracy for the modes of composite dielectric waveguides with arbitrary cross-sections and substrate layers. The STMBIE can handle both corners and junctions without loss of accuracy due to only involving operators with weakly-singular kernels. The STMBIE method significantly outperforms both FD and FE methods in accuracy, CPU time, and memory required, making the approach appealing for EM engineering applications.

The present STMBIE mode solver can be integrated as an incident excitation with full-wave solvers for nonuniform waveguide problems—either using volumetric [10] or surface BIE [11], [12] methods. Furthermore, together with efficient optimization techniques [13], complex nanophotonic devices with input/output waveguide modes can be designed.

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REFERENCES

[1] D. Song and Y. Y. Lu, "Pseudospectral modal method for computing optical waveguide modes," *Journal of Lightwave Technology*, vol. 32, no. 8, pp. 1624–1630, 2014.

[2] W. Lu and Y. Y. Lu, "Waveguide mode solver based on Neumann-to-Dirichlet operators and boundary integral equations," *Journal of Computational Physics*, vol. 231, no. 4, pp. 1360–1371, 2012.

[3] X. Claeys, R. Hiptmair, and E. Spindler, "Second-kind boundary integral equations for electromagnetic scattering at composite objects," *Computers & Mathematics with Applications*, vol. 74, no. 11, pp. 2650–2670, 2017.

[4] C. Jerez-Hanckes, C. Pérez-Arancibia, and C. Turc, "Multitrace/singletrace formulations and domain decomposition methods for the solution of Helmholtz transmission problems for bounded composite scatterers," *Journal of Computational Physics*, vol. 350, pp. 343–360, 2017.

[5] C. Müller, *Foundations of the mathematical theory of electromagnetic waves*. Springer Science & Business Media, 2013, vol. 155.

[6] J. Lai and S. Jiang, "Second kind integral equation formulation for the mode calculation of optical waveguides," *Applied and Computational Harmonic Analysis*, vol. 44, no. 3, pp. 645–664, 2018.

[7] C. Pérez-Arancibia and O. P. Bruno, "High-order integral equation methods for problems of scattering by bumps and cavities on half-planes," *Journal of the Optical Society of America A*, vol. 31, no. 8, pp. 1738–1746, Aug. 2014.

[8] L. Banjai and W. Hackbusch, "Hierarchical matrix techniques for low-and high-frequency helmholtz problems," *IMA Journal of Numerical Analysis*, vol. 28, no. 1, pp. 46–79, 2008.

[9] L. Greengard, Jingfang Huang, V. Rokhlin, and S. Wandzura, "Accelerating fast multipole methods for the Helmholtz equation at low frequencies," *IEEE Computational Science and Engineering*, vol. 5, no. 3, pp. 32–38, 1998.

[10] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed. Norwood: Artech House, Inc., 2005.

[11] O. P. Bruno, E. Garza, and C. Pérez-Arancibia, "Windowed Green function method for nonuniform open-waveguide problems," *IEEE Transactions on Antennas and Propagation*, vol. 65, no. 9, pp. 4684–4692, 2017.

[12] L. Zhang, J. H. Lee, A. Oskooi, A. Hochman, J. K. White, and S. G. Johnson, "A novel boundary element method using surface conductive absorbers for full-wave analysis of 3-D nanophotonics," *Journal of Lightwave Technology*, vol. 29, no. 7, pp. 949–959, apr 2011.

[13] C. Sideris, E. Garza, and O. P. Bruno, "Ultrafast simulation and optimization of nanophotonic devices with integral equation methods," *ACS Photonics*, vol. 6, no. 12, pp. 3233–3240, 2019. [Online]. Available: https://doi.org/10.1021/acsphotonics.9b01137