Analysis of Photonic-Crystal Problems with MLFMA and Approximate Schur Preconditioners

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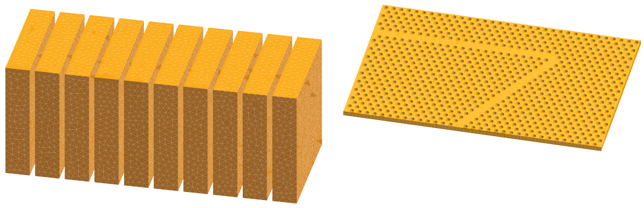
***Abstract*—We consider fast and accurate solutions of electromagnetics problems involving three-dimensional photonic crystals (PhCs). Problems are formulated with the combined tangential formulation (CTF) and the electric and magnetic current combined-field integral equation (JMCFIE) discretized with the Rao-Wilton-Glisson functions. Matrix equations are solved iteratively by the multilevel fast multipole algorithm. Since PhC problems are difficult to solve iteratively, robust preconditioning techniques are required to accelerate iterative solutions. We show that novel approximate Schur preconditioners enable efficient solutions of PhC problems by reducing the number of iterations significantly for both CTF and JMCFIE.**



(a) (b)

Fig. 1. Two types of PhC problems considered in this paper; (a) periodic slabs and (b) perforated PhC waveguide.

I. Introduction

Photonic crystals (PhCs) are artificial structures, which are usually constructed by periodically arranging dielectric unit cells, such as periodic slabs and a perforated PhC waveguide depicted in Fig. 1. Those structures exhibit frequency-selective electromagnetic responses, i.e., their electromagnetic transmission properties change rapidly as a function of frequency. For example, the PhC structure involving periodic rectangular slabs in Fig. 1(a) is usually transparent, but it becomes opaque and inhibits the transmission of electromagnetic waves in some frequency bands [1]. This structure can be used as a filter in microwave circuits and antenna systems. The perforated PhC structure in Fig. 1(b) is also frequency-selective, and it can be used as an efficient waveguide to change the direction of electromagnetic waves [2].

In this study, we consider fast and accurate solutions of electromagnetics problems involving three-dimensional PhCs, such as depicted in Fig. 1. Problems are formulated with the combined tangential formulation (CTF) [3] and the electric and magnetic current combined-field integral equation (JMCFIE) [4], discretized with the Rao-Wilton-Glisson (RWG) functions [5]. Matrix equations are solved iteratively using the multilevel fast multipole algorithm (MLFMA) [6], and iterative solutions are accelerated via novel approximate Schur preconditioners (ASPs). We extensively investigate solutions of PhC problems in terms of accuracy and efficiency. We show that ASPs reduce the number of iterations significantly for both CTF and JMCFIE.

II. Surface Formulations for Dielectric Problems

In the literature, various dielectric formulations are available for the solution of dielectric problems. Among many choices, CTF and JMCFIE are usually most suitable formulations in terms of accuracy and efficiency [7]. CTF is a modified and more stable version of the well-known Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation [3]. This formulation is practically a first-kind integral equation, and it produces ill-conditioned matrix equations without preconditioning. Nevertheless, accuracy of CTF is excellent, even when it is discretized with low-order basis functions, such as the RWG functions. On the other hand, JMCFIE is a second-kind integral equation and it usually produces better-conditioned matrix equations compared to CTF. Unfortunately, the accuracy of JMCFIE can be poor, especially when it is discretized with low-order basis functions, due to the excessive discretization error of the identity operator [8]. In addition, the accuracy of JMCFIE further deteriorates as the contrast of the object increases and/or the object involves sharp edges and corners [9].

Discretizations of integral-equation formulations for homogeneous objects lead to $2N \times 2N$ dense matrix equations in the form of

$$\begin{bmatrix} \bar{\boldsymbol{Z}}_{11} & \bar{\boldsymbol{Z}}_{12} \\ \bar{\boldsymbol{Z}}_{21} & \bar{\boldsymbol{Z}}_{22} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{a}_J \\ \boldsymbol{a}_M \end{bmatrix} = \begin{bmatrix} \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \end{bmatrix}, \text{ or } \bar{\boldsymbol{Z}} \cdot \boldsymbol{a} = \boldsymbol{v}, \quad (1)$$

where $\bar{\boldsymbol{Z}} \in \mathbb{C}^{2N\times 2N}$ and $\bar{\boldsymbol{Z}}_{11}, \bar{\boldsymbol{Z}}_{12}, \bar{\boldsymbol{Z}}_{21}, \bar{\boldsymbol{Z}}_{22} \in \mathbb{C}^{N\times N}$. Solutions of (1) via Krylov-subspace algorithms provide expansion coefficients $\boldsymbol{a}_J$ and $\boldsymbol{a}_M$ for equivalent electric and

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magnetic currents, respectively. Using expansion coefficient, scattered electric and magnetic fields can be calculated everywhere.

Matrix-vector multiplications (MVMs) required by iterative algorithms can be performed efficiently with $\mathcal{O}(N \log N)$ complexity using MLFMA. This method is based on the calculation of interactions between basis and testing functions in a group-by-group manner in a multilevel scheme. In the case of dielectric problems, MLFMA must be applied for both inner and outer media [7].

III. Approximate Schur Preconditioners

Both CTF and JMCFIE lead to non-hermitian and indefinite systems, whose iterative solutions may not converge easily without preconditioning. Being a second-kind integral equation, JMCFIE leads to diagonally-dominant matrices so that simple block-diagonal preconditioners can be effective [7]. However, CTF does not provide diagonally-dominant matrices, and its efficient solutions may require strong preconditioners constructed from all available interactions in MLFMA, i.e., near-field matrices.

Preconditioning techniques for systems similar to (1) are usually studied in the context of generalized-saddle-point problems [10]–[15]. Approximating the dense matrix in (1) by a sparse near-field matrix $\bar{\boldsymbol{Z}}^{NF}$, preconditioners developed for saddle-point problems can be used for integral-equation solutions of dielectric problems. In general, those preconditioners are obtained with some approximations to the Schur complement reduction, which decomposes the solution of a 2×2 partitioned near-field system

$$\begin{bmatrix} \bar{\boldsymbol{Z}}_{11}^{NF} & \bar{\boldsymbol{Z}}_{12}^{NF} \\ \bar{\boldsymbol{Z}}_{21}^{NF} & \bar{\boldsymbol{Z}}_{22}^{NF} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}, \tag{2}$$

into solutions of two systems, i.e.,

$$\bar{\boldsymbol{Z}}_{11}^{NF} \cdot \boldsymbol{x} = \boldsymbol{f} - \bar{\boldsymbol{Z}}_{12}^{NF} \cdot \boldsymbol{y} \tag{3}$$

$$\bar{\boldsymbol{S}} \cdot \boldsymbol{y} = \boldsymbol{g} - \bar{\boldsymbol{Z}}_{21}^{NF} \cdot \left(\bar{\boldsymbol{Z}}_{11}^{NF}\right)^{-1} \cdot \boldsymbol{f}, \tag{4}$$

where

$$\bar{\boldsymbol{S}} = \bar{\boldsymbol{Z}}_{22}^{NF} - \bar{\boldsymbol{Z}}_{21}^{NF} \cdot \left(\bar{\boldsymbol{Z}}_{11}^{NF}\right)^{-1} \cdot \bar{\boldsymbol{Z}}_{12}^{NF}. \tag{5}$$

Success of those preconditioners depend on fast and efficient solutions of (3) and (4). Hence, we need effective approximations to the inverse of $\bar{\boldsymbol{Z}}_{11}^{NF}$, as well as the inverse of $\bar{\boldsymbol{S}}$.

One can use the sparse-approximate inverse (SAI) of $\bar{\boldsymbol{Z}}_{11}^{NF}$, i.e.,

$$\bar{\boldsymbol{M}}_{11} \approx \left[\bar{\boldsymbol{Z}}_{11}^{NF}\right]^{-1}, \tag{6}$$

in (4) and (5). Then, the solution of (3) can be written as

$$\boldsymbol{x} \approx \bar{\boldsymbol{M}}_{11} \cdot \left(\boldsymbol{f} - \bar{\boldsymbol{Z}}_{12}^{NF} \cdot \boldsymbol{y}\right). \tag{7}$$

However, a good approximation to $\boldsymbol{y}$ is required in (7). Consequently, we also need to develop a good approximation to the Schur complement matrix.

We note that, in many applications involving partitioned systems, the partition $\bar{\boldsymbol{Z}}_{22}^{NF}$ is identically zero, or it consists of very small elements compared to elements in other partitions [10]. Unfortunately, this is not valid for matrix equations obtained from CTF and JMCFIE, and we are unable use many techniques developed for those cases in the literature. In our case, an applicable method can be using a Krylov-subspace solver to obtain an approximate solution of the system in (4). MVMs with $\bar{\boldsymbol{S}}$ can be performed by approximating the inverse of $\bar{\boldsymbol{Z}}_{11}^{NF}$ with $\bar{\boldsymbol{M}}_{11}$. However, a robust preconditioner for $\bar{\boldsymbol{S}}$ is still required.

One option is to ignore the second term in (5) and to approximate the inverse of the Schur complement by $\bar{\boldsymbol{M}}_{22}$, i.e., SAI of $\bar{\boldsymbol{Z}}_{22}^{NF}$. For both CTF and JMCFIE, $\bar{\boldsymbol{Z}}_{22}^{NF} = \bar{\boldsymbol{Z}}_{11}^{NF}$, hence $\bar{\boldsymbol{M}}_{11}$ can also provide an approximation to the inverse of the Schur complement $\bar{\boldsymbol{S}}$. Hence, one can find an approximation to $\boldsymbol{y}$ as

$$\boldsymbol{y} \approx \bar{\boldsymbol{M}}_{11} \cdot \left(\boldsymbol{g} - \bar{\boldsymbol{Z}}_{21}^{NF} \cdot \bar{\boldsymbol{M}}_{11} \cdot \boldsymbol{f}\right), \tag{8}$$

which can be used in (7). We call the resulting preconditioner defined by (7) and (8) as ASP. $\bar{\boldsymbol{M}}_{11}$ can also be used as a preconditioner for iterative solutions of (3) and (4), provided that $\bar{\boldsymbol{M}}_{11}$ is used instead of exact inverses in (5) and (4). In this case, the preconditioner is called iterative ASP (IASP). We note that a flexible solver is required for IASP since the effective preconditioner changes from iteration to iteration [16]. Finally, if $\bar{\boldsymbol{M}}_{11}$ does not provide a good approximation to $\bar{\boldsymbol{S}}$, a better approximation to the inverse of the Schur complement can be obtained via incomplete MVMs, as detailed in [17].

TABLE I
PhC Problems

PERIODIC SLABS			
Problem	Slab Size (m)	Number of Walls	Unknowns
S1	0.41×2×2	5	38,700
S2	0.41×2×2	10	77,400
S3	0.41×4×4	5	131,460
S4	0.41×4×4	10	262,920
PERFORATED PhC WAVEGUIDE			
Problem	Size (cm)	Number of Holes	Unknowns
P1	0.6×5×5	18	14,226
P2	0.6×5×10	38	27,798
P3	0.6×15×20	272	162,420
P4	0.6×26×34	828	475,782

IV. Results

Table I lists PhC problems involving periodic slabs and perforated PhC waveguides considered in this paper. All structures are located in free space and illuminated by a Hertzian dipole. The relative permittivity of PhCs involving periodic slabs is 4.8, and they are expected to resonate at 300 MHz. Those structures are investigated at 250 MHz, 300 MHz, and 350 MHz. Perforated PhC waveguides have relative permittivities of 12.0 and they are investigated at 8.25 GHz, i.e., at the frequency for the most efficient transmission. Problems are formulated with both CTF and JMCFIE. Periodic slabs are discretized with $\lambda/10$ triangles, where λ is the wavelength in free space. Perforated PhC slabs require finer triangulations with $\lambda/20$ triangles for accurate modelling of air holes.

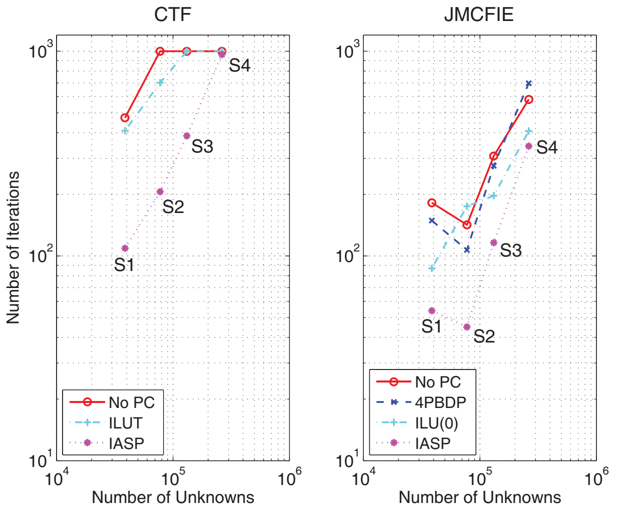

Fig. 2. Number of iterations for the solution of periodic-slab problems listed in Table I.

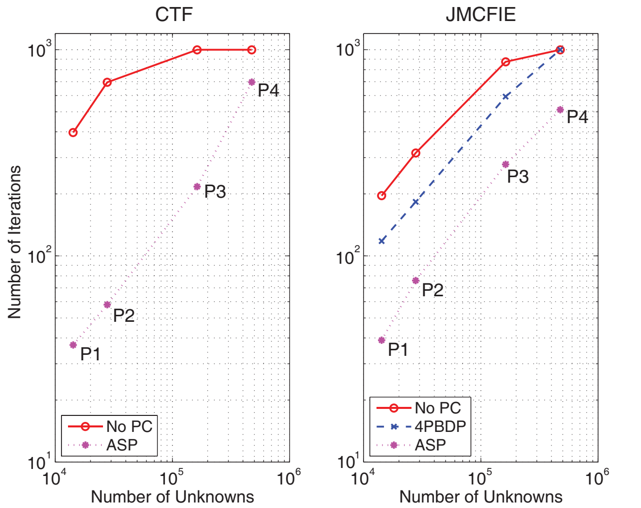

Fig. 3. Number of iterations for the solution of perforated-PhC problems listed in Table I.

Iterative solutions are performed by the generalized-minimal-residual (GMRES) method [16] without a restart. The relative residual error for the convergence is set to 10^{-3}. Iterations are started with a zero initial guess and terminated at maximum 1000th iteration.

Fig. 2 depicts the solution of periodic-slab problems at 300 MHz. We compare iteration counts when solutions are accelerated with a four-partition block-diagonal preconditioner (4PBDP) [7], ILU-type preconditioners (ILU(0) for JMCFIE and ILUT for CTF) [16]), and IASP, in addition to the no-preconditioner (NP) case. Solutions employing 4PBDP are omitted for CTF since they do not converge. In addition, CTF solutions do not converge for large problems without preconditioning or when using ILU(0). In the case of IASP, we use only $\bar{\boldsymbol{M}}_{11}$ as the inner preconditioner so that the amount of memory required by this preconditioner is 1/4 of that of ILU-type preconditioners. Fig. 2 shows that IASP provides the most efficient solutions of periodic-slab problems.

Fig. 3 depicts the solution of perforated-PhC problems. In this case, we omit ILU-type preconditioners since their memory requirement is excessively large for the largest two problems. In addition, 4PBDP is again omitted for CTF due to nonconvergent solutions. Fig. 3 shows that ASP, which employs incomplete MVMs, significantly accelerates iterative solutions of CTF. ASP is also very effective for JMCFIE and reduces the number of iterations significantly, compared to solutions without preconditioning and with 4PBDP. We note that the largest problem in Fig. 3 cannot be solved without using ASP.

Fig. 4 presents power transmission results for the periodic-slabs problem S2. The power transmission is calculated point-wise around dielectric slabs, and the transmission properties of the structure is investigated at 250 MHz, 300 MHz, and 350 MHz. We observe that the structure is transparent at 250 MHz and 350 MHz, i.e., the power transmission is unity in the transmission region on the left-hand side of the structure. At 300 MHz, however, the structure becomes opaque and a shadowing occurs. We also note that there are discrepancies between results obtained by using CTF and JMCFIE; this is mostly due to the inaccuracy of JMCFIE.

Fig. 5 presents near-zone magnetic fields for the perforated-PhC problem P4. The total magnetic field is calculated point-wise inside and outside the structure in order to demonstrate the transmission of electromagnetic waves from the left-hand side to the bottom. For this problem, we observe that results obtained by using CTF and JMCFIE are significantly different. This is due to the deteriorating accuracy of JMCFIE in the case of complicated structures and relatively high contrasts.

Finally, in order to show that the inconsistency between CTF and JMCFIE results is due to the inaccuracy of JMCFIE, we consider the solution of an electromagnetics problem involving a 0.6 cm $\times$ 7 cm $\times$ 10 cm perforated PhC waveguide. The problem is formulated with CTF and JMCFIE discretized by using $\lambda/20$ and $\lambda/40$ triangles. Fig. 6 presents the magnetic field at 8.25 GHz. We observe that results obtained by JMCFIE change drastically when the discretization is refined. Specifically, JMCFIE results become consistent with CTF results for the dense discretization.

V. Concluding Remarks

In this paper, we consider MLFMA solutions of electromagnetics problems involving three-dimensional PhCs formulated with CTF and JMCFIE. In addition to MLFMA, robust preconditioning techniques are required in order to solve PhC problems efficiently. We show that novel ASPs accelerate iterative solutions significantly and they enable the analysis of relatively large PhC structures.

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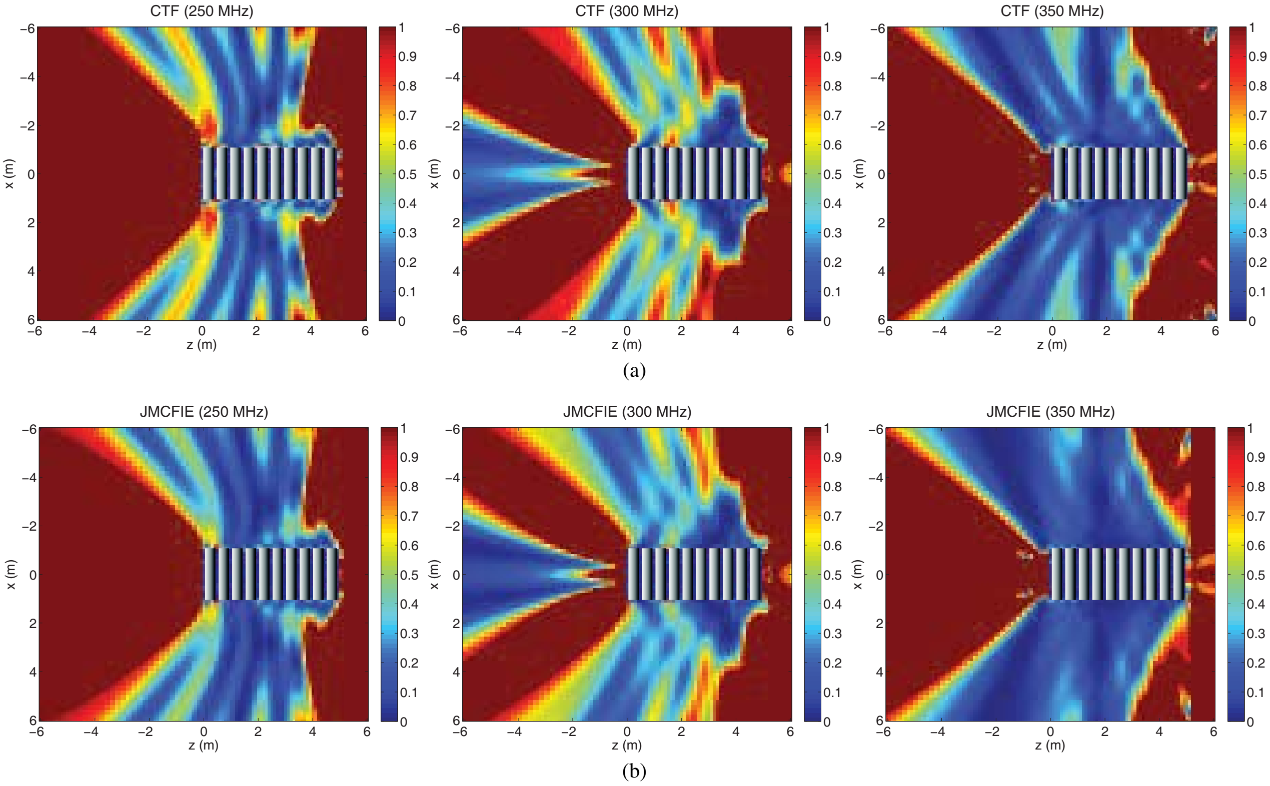

Fig. 4. Power transmission for a PhC involving periodic slabs (S2 in Table I) at 250 MHz, 300 MHz, and 350 MHz, obtained by using (a) CTF and (b) JMCFIE.

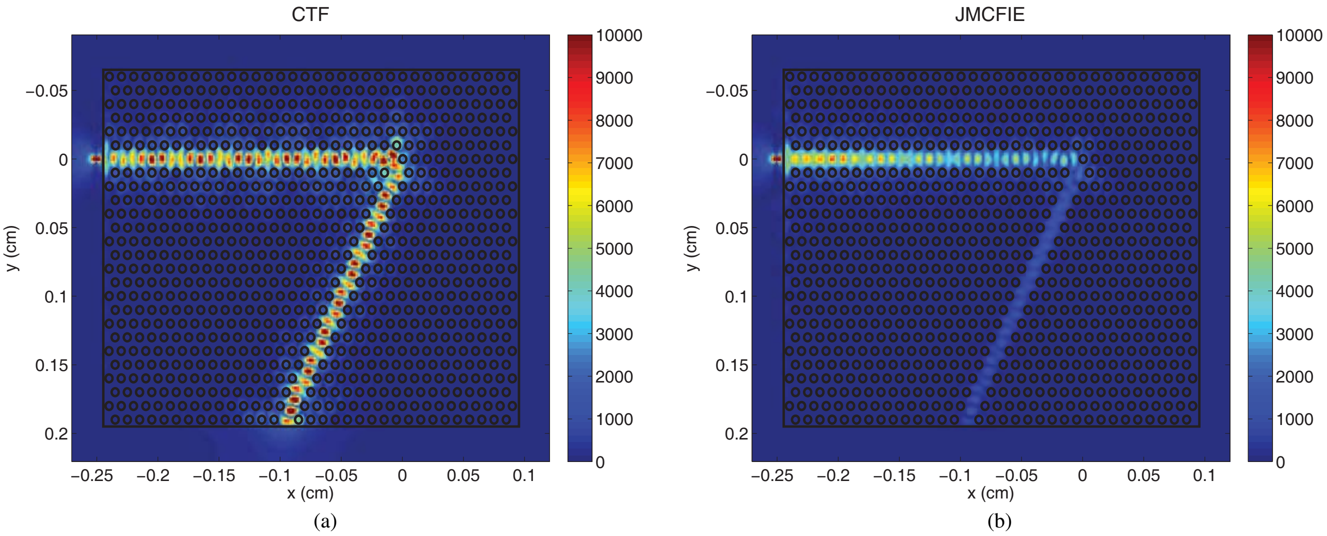

Fig. 5. Near-zone magnetic fields for a perforated PhC waveguide (P4 in Table I) illuminated by a Hertzian dipole radiating from $x = -0.25$ cm. The problem is formulated with (a) CTF and (b) JMCFIE.

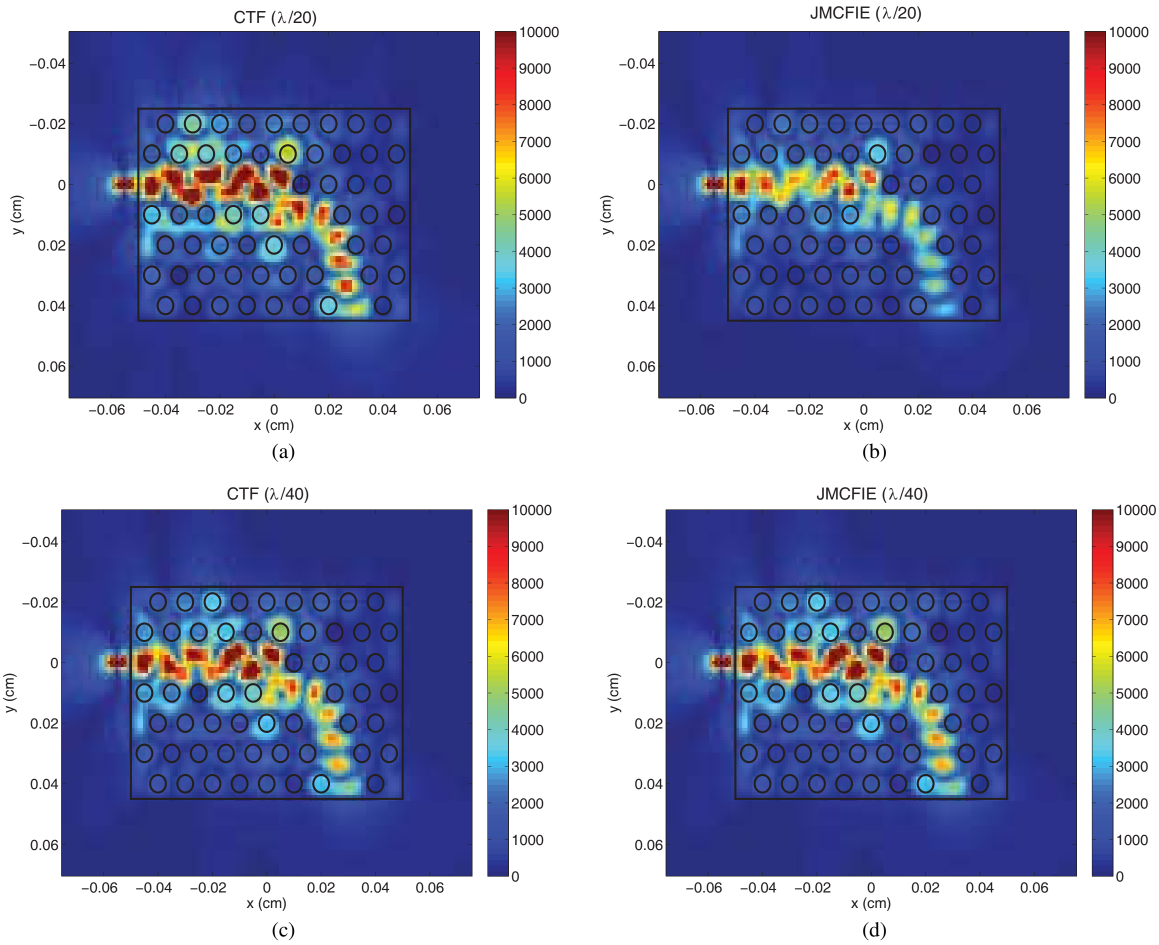

Fig. 6. Near-zone magnetic fields for a perforated PhC waveguide involving 7×10 holes illuminated by a Hertzian dipole. Solutions are obtained with (a) CTF and $\lambda/20$ triangulation, (b) JMCFIE and $\lambda/20$ triangulation, (c) CTF and $\lambda/40$ triangulation, and (d) JMCFIE and $\lambda/40$ triangulation.

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