A 2.5-D Scalar Helmholtz Wave Solution Employing the Spectral Lanczos Decomposition Method (SLDM)†

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Abstract

A numerical method is derived for obtaining the solution to the 2.5-D scalar Helmholtz equation involving an arbitrary 2-D lossless inhomogeneous dielectric scatterer excited by a point source in a closed waveguide. The spectral Lanczos decomposition method (SLDM) is used to solve the differential equation by polynomial approximation. Numerical results indicate that a convergent solution to the 2.5-D problem in a bounded region may be achieved in $O(N^{1.5})$ operations, in agreement with a theoretical upper bound of $O(N^{1.5}\log N)$. Also, it is demonstrated that the method is accurate for resonant solutions involving eigenvalues on the order of the machine precision. Extension to lossy dielectrics and the implementation of an absorbing boundary condition is discussed.

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1. Introduction

The Lanczos method was presented by Lanczos [1] in 1950 as an efficient method of computing the eigenpairs of a large sparse symmetric matrix. The method has suffered due to numerical instabilities whereby the eigenvectors produced by the Lanczos process lose their orthogonality as the algorithm progresses and spurious repeated eigenvalues are produced. But in 1971, Paige showed that despite the numerical errors, reliable results are achievable [2]. In what has become known as the "Lanczos phenomenon," Paige showed that if the Lanczos process is carried out far enough, eventually all of the eigenvalues of the original matrix will appear as eigenvalues of the tridiagonal matrix produced by the Lanczos process (see also [3] and [4]).

The idea behind the spectral Lanczos decomposition method (SLDM) proposed by Druskin and Knizhnerman [5, 6] is to use the Lanczos method to build up orthogonal polynomials that approximate the solution to a differential equation. Previously, Lanczos methods were used to calculate the solution to one-dimensional [7] and multi-dimensional [8] parabolic and hyperbolic problems. Methods similar to the SLDM approach were used in computational chemistry to calculate spin relaxations in molecular dynamics [9] and also in [10].

Recently, it was shown by Allers, Sezginer and Druskin [11] and also by Tamarchenko [12] that the SLDM technique may be used to solve the 2.5-D Laplace equation efficiently. The 2.5-D problem is characterized by an inhomogeneity that varies in two spatial dimensions, but fields must be computed in three dimensions because the source is localized in 3-D. The advantage to using the SLDM here is that the z-variation may be computed analytically and numerical computations only need to be performed in a 2-D plane.

We consider here the extension of the 2.5-D SLDM to the scalar Helmholtz equation for an arbitrary lossless dielectric scatterer. Several difficulties naturally arise because the propagation matrix is no longer definite and hence contains both positive and negative eigenvalues corresponding to propagating and evanescent modes. One problem is that we do not have a general proof of convergence for the indefinite case as we do for a definite matrix (see [5] and [6]). However, certain convergence proofs for the definite case may be extended for bounded problems where there are relatively few propagating eigenvalues [13]. Our computer results indicate that convergence for the bounded problem can be achieved in $M \sim O(\sqrt{N})$ steps of the Lanczos process for an $N \times N$ matrix, yielding a 2.5-D solution in $O(N^{1.5})$ floating-point operations.

Another issue is the question of the accuracy of the method in the presence of very small eigenvalues. We demonstrate using a computer simulation that we can recover small eigenvalues on the order of the machine precision and therefore obtain an accurate solution near resonance. Problems involving a resonant solution with precisely zero eigenvalue are not solvable using this method.

The numerical example that we use to demonstrate the method consists of the computation of the point source response in a rectangular waveguide with a Dirichlet boundary condition. Comparison is made between the SLDM solution and closed-form solutions for both a continuous and discretized waveguide. Finally, we discuss the addition of lossy dielectrics and the implementation of an absorbing boundary condition in order to extend the method to wave scattering problems in an unbounded homogeneous background.

2. SLDM Solution

The 2.5-D scalar wave equation for a planar source may be written as

$$\left[\nabla_s^2 + \frac{\partial^2}{\partial z^2} + \frac{\omega^2}{c^2(\boldsymbol{\rho})}\right] \phi(\boldsymbol{\rho}, z) = s(\boldsymbol{\rho})\delta(z), \tag{1}$$

which becomes

$$\left[\nabla_s^2 + \frac{\omega^2}{c^2(\boldsymbol{\rho})} - k_z^2\right] \phi(\boldsymbol{\rho}, k_z) = s(\boldsymbol{\rho}) \tag{2}$$

after a Fourier transform is applied in the z variable. Discretizing the above, we may rewrite Equation (2) as

$$\left(\overline{\boldsymbol{D}}_s + \overline{\boldsymbol{C}} - \Delta^2 k_z^2 \overline{\boldsymbol{I}}\right) \boldsymbol{\phi}(k_z) = \Delta^2 \boldsymbol{s} \tag{3}$$

where

$$C_{jk} = \frac{\Delta^2 \omega^2}{c^2(\rho_j)} \delta_{jk}, \tag{4}$$

and $\overline{\boldsymbol{D}}_s$ is the normalized discrete 2-D Laplacian operator. For elements j interior to the finite difference grid, $\overline{\boldsymbol{D}}_s$ has the form

$$\left[\overline{\boldsymbol{D}}_s \cdot \boldsymbol{\phi}\right]_j = \phi_{j+1} + \phi_{j-1} + \phi_{j+n_y} + \phi_{j-n_y} - 4\phi_j \tag{5}$$

where n_y is the number of discretization points in the y dimension.

Now we let $\overline{\boldsymbol{A}} = \overline{\boldsymbol{D}}_s + \overline{\boldsymbol{C}}$ and write the solution to Equation (3) for a particular value of k_z as

$$\boldsymbol{\phi}(k_z) = \Delta^2 \left(\overline{\boldsymbol{A}} - \Delta^2 k_z^2 \; \overline{\boldsymbol{I}}\right)^{-1} \cdot \boldsymbol{s}. \tag{6}$$

We assume throughout this paper that the inhomogeneous medium is lossless, giving rise to a sparse real symmetric $N \times N$ matrix $\overline{\boldsymbol{A}}$. Forming the spectral Lanczos decomposition of $\overline{\boldsymbol{A}}$,

$$\overline{\boldsymbol{A}} \cdot \overline{\boldsymbol{Q}} = \overline{\boldsymbol{Q}} \cdot \overline{\boldsymbol{T}} \tag{7}$$

where $\overline{\boldsymbol{T}}$ is the $M \times M$ tridiagonal Lanczos matrix and $\overline{\boldsymbol{Q}} = [\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_M]$ is the matrix containing the Lanczos vectors. The Lanczos process is started with the choice

$$\boldsymbol{q}_1 = \overline{\boldsymbol{Q}} \cdot \boldsymbol{e}_1 = \boldsymbol{s}/\|\boldsymbol{s}\|. \tag{8}$$

Taking the spectral decomposition of the tridiagonal matrix $\overline{\boldsymbol{T}}$, we have

$$\overline{\boldsymbol{T}} = \overline{\boldsymbol{V}} \cdot \overline{\boldsymbol{\Lambda}} \cdot \overline{\boldsymbol{V}}^{\,t} \tag{9}$$

where $\overline{\boldsymbol{\Lambda}} = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_M]$. Using the above, Equation (6) may be rewritten as

$$\boldsymbol{\phi}(k_z) = \Delta^2 \|\boldsymbol{s}\| \overline{\boldsymbol{Q}} \cdot \overline{\boldsymbol{V}} \cdot \left(\overline{\boldsymbol{\Lambda}} - k_z^2 \Delta^2 \; \overline{\boldsymbol{I}}\right)^{-1} \cdot \overline{\boldsymbol{V}}^{\,t} \cdot \boldsymbol{e}_1. \tag{10}$$

Note that the manipulations leading up to Equation (10) do not depend on the orthogonality of the Lanczos vectors $\boldsymbol{q}_i, \quad i = 1, 2, \ldots, M$. We believe that this is one of the main reasons that the SLDM gives accurate results in spite of the loss of orthogonality caused by numerical errors in the Lanczos process.

Finally, we perform the inverse Fourier transform of Equation (10) by extending the integral into the complex plane and applying a contour integration. We have the result

$$[\boldsymbol{\phi}(z)]_j = \frac{-i\Delta\|\boldsymbol{s}\|}{2} \sum_{k=1}^{M} Q_{jk} \sum_{m=1}^{M} V_{km} V_{1m} \lambda_m^{-1/2} e^{\pm i\lambda_m^{1/2} z/\Delta}, \quad z \gtrless 0. \tag{11}$$

Note that the computation of the matrix-vector product $\overline{\boldsymbol{A}} \cdot \boldsymbol{q}$ in the Lanczos process here is an $O(N)$ operation because $\overline{\boldsymbol{A}}$ is sparse. If the Lanczos process is continued for $M \sim \sqrt{N}$ steps, the complexity of the method becomes $O(N^{1.5})$. The eigenvalues of the $M \times M$ tridiagonal matrix $\overline{\boldsymbol{T}}$ may be computed in $O(M^2)$ operations using the QL algorithm, but if all eigenvectors are required then computation of the eigenvectors requires $O(M^3) = O(N^{1.5})$ operations.

If one is only interested in the solution several wavelengths away from the source, only those eigenvectors corresponding to propagating modes (positive eigenvalues) and a few of the negative eigenvalues with small magnitude have to be computed. If these few eigenvectors are computed using inverse iteration, it could speed up the code considerably, but would not reduce the computational complexity below $O(N^{1.5})$.

3. Example: Point Source Response of a Rectangular Waveguide

We illustrate the technique by considering the computation of the point source response (Green's function) for a rectangular waveguide of dimension $a \times b$ with a Dirichlet boundary condition. The Green's function may be computed in closed form as

$$g(\boldsymbol{r}, \boldsymbol{r}') = \frac{2i}{ab} \sum_p \sum_q \frac{1}{k_{pq}} \sin\left(\frac{p\pi x}{a}\right) \sin\left(\frac{p\pi x'}{a}\right) \sin\left(\frac{q\pi y}{b}\right) \sin\left(\frac{q\pi y'}{b}\right) \times e^{\pm i k_{pq}(z-z')}, \quad z \gtrless z'. \tag{12}$$

The eigenvalues are given as

$$k_{pq} = \sqrt{k_0^2 - \left(\frac{p\pi}{a}\right)^2 - \left(\frac{q\pi}{b}\right)^2}, \quad p, q = 1, \ldots, \infty \tag{13}$$

for a continuous waveguide and

$$k_{pq} = \left\{ k_0^2 - \frac{4(n_x+1)^2}{a^2} \sin^2\left[\frac{p\pi}{2(n_x+1)}\right] - \frac{4(n_y+1)^2}{b^2} \sin^2\left[\frac{q\pi}{2(n_y+1)}\right] \right\}^{1/2} \tag{14}$$
$$p = 1, \ldots, n_x, \qquad q = 1, \ldots, n_y$$

for a discretized waveguide, where n_x and n_y represent the number of discretization points along the x and y axis. Note that the double summation in Equation (12) is carried out over an infinite number of modes in the continuous case, but is limited to a finite number for the discrete case.

The solution was computed for a $5.2\lambda \times 5.2\lambda$ square waveguide square waveguide using both the SLDM approach and the closed-form solution above. We used a value of $k_0 = .62832$ ($\lambda = 10$ mm) with waveguide dimensions $a = b = 52$ mm. The SLDM solution was computed for three different discretization levels: a 51×51 grid (10 points/λ), a 155×155 grid (29.8 points/λ) and a 259×259 grid (49.8 points/λ).

Figure 1 shows a comparison of the point source response computed using SLDM with the three levels of discretization versus the analytic solution for the continuous waveguide. In Figure 1(a) it is clear that the solution for the 51×51 grid does not agree well with the analytic solution. Note in particular that the error in the solution increases with z. This error is not inherent in the SLDM computation; it is a modeling error known as grid dispersion that is due to discretization of the field inside the waveguide. As the discretization density is increased in Figure 1(a), the SLDM solution approaches the analytic solution for the continuous waveguide.

Figures 1(b) and 1(c) show a cross-section of the field in the waveguide at $z = 0.8\lambda$ and $z = 3.5\lambda$. The SLDM solution for the 51×51 grid is not shown in parts (b) and (c) because the amount of grid dispersion is so high.

In Figure 2 we compare the SLDM solution to the analytic solution for a discrete waveguide. A z-axis cut for the 51×51 grid is shown in (a) and a cross-section is shown in (b) for the 155×155 grid at $z = 0.8\lambda$. The SLDM and the analytic solution for the discretized waveguide are indistinguishable. The results in Figure 2 clearly show that nearly all of the errors that appear in Figure 1 are due to grid dispersion, and not errors in the SLDM computation.

Table 1 shows a breakdown of the computation times for various parts of the SLDM solution along with memory usage and the number of steps of the Lanczos process required for convergence. The number of steps required for convergence was determined by trial-and-error here, although more systematic methods are given in [4] and [14]. We found that the value of M required for convergence was well defined since the error in the solution was quite noticeable when the solution did not converge.

The computation times reported in Table 1, with the exception of the CPU seconds reported by the operating system, are wallclock times accurate to the nearest second that were computed by averaging three trial runs of the code. The code was run on a Convex C-240 supercomputer with 4 processors, 512 MB of RAM and 12 GB of disk space. The row "Memory Required" in Table 1 was for temporary storage of the Lanczos vectors in the $\overline{\boldsymbol{Q}}$ matrix. These vectors were written temporarily to disk and read back in for the field computation. This operation of writing/reading the vectors to disk (reported as "Time Using I/O") appears to be the main bottleneck in the code and could probably be reduced. Apparently this disk swapping was unnecessary here since the CPU had enough RAM to contain all of the Lanczos vectors.

4. Discussion on Convergence of the Method

Note from Table 1 that we were able to achieve convergence of the method using $2\sqrt{N} < M < 2.5\sqrt{N}$. While there are no general convergence proofs in existence for the indefinite problem, a recent analysis [13] indicates that for bounded problems where there are only a relatively few propagating eigenmodes, the convergence is asymptotically the same as for the definite case as $N \to \infty$. By equating the grid dispersion error with the SLDM error, we can then derive a theoretical upper bound of $M < \sqrt{N}\ \log N$. This $\log N$ factor was not observed in our computer simulation results because $\log N$ grows slowly compared to $\sqrt{N}$ and our stopping criterion was somewhat arbitrary.

The convergence is also assisted here by the grid dispersion requirements. From Equation (14), we can show that a zero eigenvalue in the center of the spectrum would require a grid density of $\Delta = a/(n_x + 1) = b/(n_y + 1) = \lambda/\pi$ (comparing Equations (11) and (12) it is obvious that $\lambda_m = \Delta^2 k_{pq}^2$). However, grid dispersion requirements usually dictate a grid density on the order of $\Delta = \lambda/30$. This has the effect of causing most of the eigenvalues for the discrete problem to be evanescent and pushing the relatively few propagating eigenvectors to the outside of the spectrum. But we warn that the evanescence is in z and consequently, all of the eigenvalues and eigenvectors are important if one is interested in the coplanar solution with $z = 0$. Similarly, the effect may not be present when absorbing boundaries are added.

To demonstrate that the method is accurate for computing very small eigenvalues, we simulated two cases of near zero eigenvalues with a 51×51 grid. The first case consisted of choosing a value of k_0 near that used in the numerical example. Table 2 shows the values of k_0 used along with the true eigenvalue, the eigenvalue obtained from SLDM, and the value of M required for convergence. It is clear that small eigenvalues down to approximately 100 times the machine precision (2.22×10^{-16} here) may be recovered accurately without significantly increasing M beyond that required for the non-resonant solution.

Next, we simulated the case of a near zero eigenvalue in the center of the spectrum by choosing a value of $k_0 = 2.0 + \delta$ for the 51×51 grid-point waveguide. From Equation (14), a zero eigenvalue occurs in the center of the spectrum for $\delta = 0$. But for $\delta \neq 0$, the small eigenvalue is given approximately as $\lambda_m^* \approx 4\Delta^2\delta$. Table 2 compares the small eigenvalue obtained using SLDM to the true eigenvalue for two values of δ and the value of M required for convergence. Apparently, small eigenvalues may be recovered accurately here as well, but the Lanczos process takes longer to converge. Although a zero eigenvalue for a bounded problem would not occur in the center of the spectrum due to the grid dispersion requirement argument given above, the example illustrates the point that the convergence of the SLDM algorithm depends heavily on the relative location of the "important" eigenvalues in the spectrum of the matrix $\overline{\boldsymbol{A}}$.

5. Extension to Lossy Media and Implementation of an Absorbing Boundary Condition

In the SLDM method that we discussed, we have restricted our attention to the study of lossless dielectrics. For the case of lossy media, reciprocity arguments show that the matrix $\overline{\boldsymbol{A}}$ becomes complex symmetric. Apparently, the complex symmetric case can be handled easily by using the same Lanczos process and SLDM technique and defining all of the relevant quantities to be complex variables (see [14] (Chap. 6)). However, we need to add the caveat that $\overline{\boldsymbol{A}}$ must be diagonalizable for this procedure to work since it is not guaranteed in general.

The implementation of an absorbing boundary condition using a standard method such as Engquist-Majda (see [15] (p. 246)) is complicated for several reasons. One is that such a method automatically makes $\overline{\boldsymbol{A}}$ complex. Another problem is that it is difficult to make a boundary condition independent of angle with respect to the z axis since the k_z values are related to the unknown eigenvalues.

Yet another problem is that the implementation of an absorbing boundary condition appears to make $\overline{\boldsymbol{A}}$ non-symmetric in general. Although this asymmetry is entirely artificial in that reciprocity guarantees $\overline{\boldsymbol{A}}$ to be complex symmetric, it is not clear how this imposed asymmetry would affect the accuracy of the solution. Perhaps the best way to impose an absorbing boundary condition here is to use an absorbing material around the edge of the grid using the so-called "anechoic chamber boundary condition" [16].

6. Conclusions

We have demonstrated that the SLDM may be used to solve the 2.5-D scalar Helmholtz equation efficiently and with a high degree of accuracy. A grid density of at least 30 points per wavelength seems to be required in order to minimize the effects of grid dispersion. The SLDM algorithm described here could easily be extended to complex media by using a Lanczos procedure for complex symmetric matrices. Extension of the method to scattering problems with radiation boundary conditions will require absorbing boundary conditions. However, the implementation of an absorbing boundary condition using standard techniques would complicate the SLDM solution because it would most likely make the $\overline{\boldsymbol{A}}$ matrix non-symmetric as well as complex. Furthermore, it is difficult to make an absorbing boundary condition independent of k_z for this problem.

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Table 1: Computation Times for Waveguide Example

	$N = 2601$	$N = 24,025$	$N = 67,081$
Number of Lanczos Steps, M	120	340	550
$M/\sqrt{N}$	2.35	2.19	2.12
Memory Required (Mb)	2.49	65.3	295.2
Time Lanczos Process (sec)	.33	6.7	48.0
Time QL Decomposition (sec)	1.0	7.0	69.0
Time using I/O (sec)	1.0	20.3	168.0
Time Computing Fields (sec)	0.0	1.66	13.3
Total Time (sec)	2.3	35.7	298.3
CPU Seconds Reported by O.S.	2.4	34.4	138.1

Table 2: Accuracy of SLDM for Small Eigenvalues ($N = 2601$)

k_0	True Eigenvalue	SLDM Eigenvalue	M Required for Convergence
.6156262927945929	1.0×10^{-8}	$1.00000085395 \times 10^{-8}$	160
.6156262846727906	1.0×10^{-14}	$.847100907057 \times 10^{-14}$	180
2.00000001	4.0×10^{-8}	$3.99999987557 \times 10^{-8}$	650
2.00000000000001	4.0×10^{-14}	$3.88658103677 \times 10^{-14}$	700

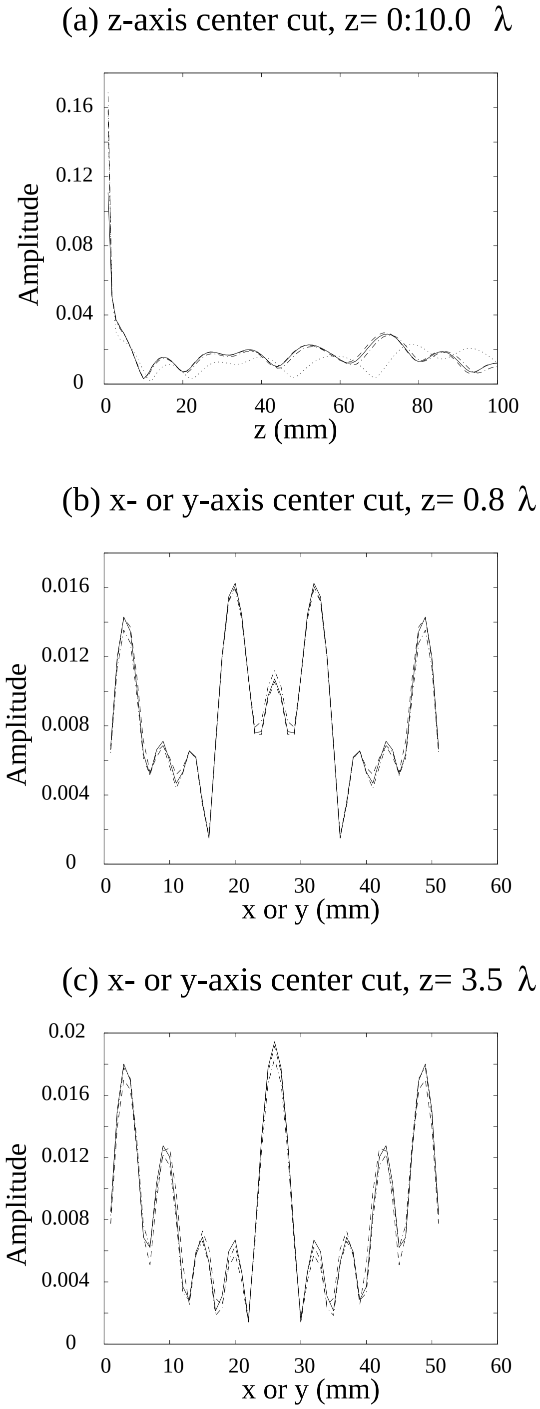

Figure 1: Point-source response for a square waveguide of dimension 52.0 mm $\times$ 52.0 mm with $\lambda = 10.0$ mm. In all figures, the solid curve is the analytic solution for a continuous waveguide, dotted curve (shown only in (a)) is SLDM solution for a 51×51 grid, dash-dot curve is SLDM solution for a 155×155 grid, dashed curve is 259×259 grid. Nearly all of the error between the SLDM solutions and the continuous analytic solution is due to grid dispersion and not errors in the SLDM method (see Figure 2).

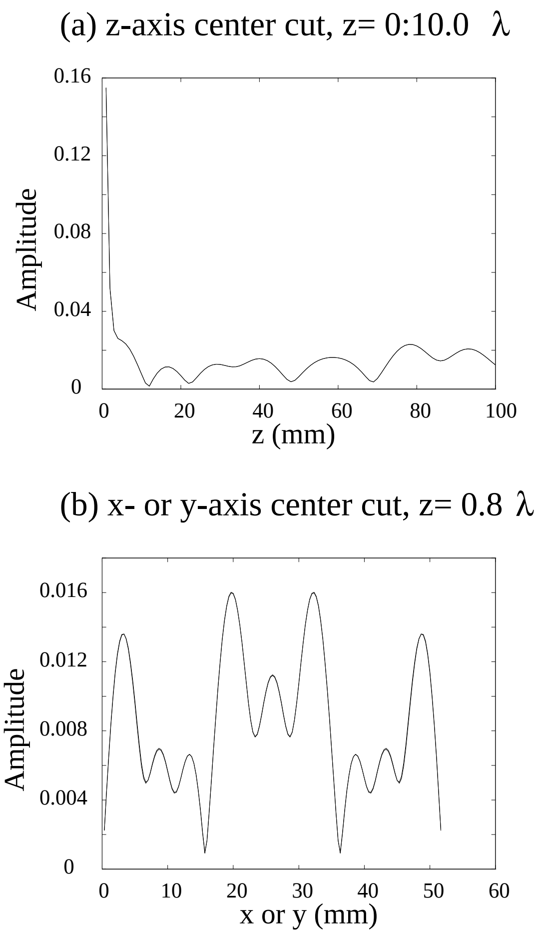

Figure 2: Comparison of SLDM solution with analytic solution for a discretized waveguide. In (a), z-axis cut for 51×51 grid is shown and in (b) x- or y-axis cut for 155×155 grid at $z = 0.8\lambda$ is shown. In both (a) and (b), SLDM solution and analytic solution for discretized waveguide are overlaid on top of each other, both using a solid line. The curves for the SLDM solution and the analytic solution are barely distinguishable, indicating excellent agreement.