Proceedings of the National Institute for Mathematical Sciences
Vol. 3, No. 9(2008), pp.65–70

COMPUTING DIRICHLET-TO-NEUMANN MAPS FOR NUMERICAL SIMULATION OF PHOTONIC CRYSTAL STRUCTURES

YA YAN LU

Abstract. Photonic crystals (PhCs) have promising applications in future integrated circuits based on lightwaves. A typical PhC structure or device has many identical unit cells. Based on the Dirichlet-to-Neumann maps of the unit cells, we have developed efficient numerical methods for analyzing various PhC structures. In this paper, these works are briefly reviewed.

1. Introduction

Photonic crystals (PhCs) [1] are periodic structures with a period on the same scale as the wavelength of light. They are being intensively studied since they allow us to control and manipulate light at a very small length scale. One of the most important properties of a PhC is the existence of special frequency intervals called bandgaps. Light cannot propagate in the PhC, if its frequency is in a bandgap. PhCs also have unusual dispersion properties leading to interesting physical phenomena such as superprism, ultrarefraction and negative refraction. Based on bandgap effect, light can be trapped in a small cavity or be forced to propagate along a waveguide when the periodicity of the PhC is intensionally broken by point or line defects.

Modeling and simulation of PhCs give rise to a number of interesting and challenging mathematical problems. The governing equations for light waves in PhCs are the Maxwell's equations. Simulations of PhCs have been carried out in either time domain or frequency domain. In the time domain, the most widely used method is the finite difference method originally proposed by Yee. Many important problems are more naturally formulated in the frequency domain. Furthermore, frequency domain methods can more easily take advantage of the special geometry features available in PhC structures.

A PhC device, created by introducing various defects in an otherwise perfectly periodic PhC, can cover many wavelengths in each direction and have thousands of unit cells, but it typically has only two or three distinct unit cell (the regular and defect cells). This is a rather obvious geometric feature that we should take advantage of. Recently, we developed a Dirichlet-to-Neumann (DtN) map method for analyzing various PhC problems. For a unit cell Ω, the DtN map is the operator Λ satisfying $\Lambda u = \partial_\nu u$ on $\partial\Omega$ (the boundary of Ω) for any u satisfying the Maxwell's equations (or simplifications) in Ω, where ν is a unit normal vector of $\partial\Omega$. More specifically, we used DtN maps to solve eigenvalue problems related to bandgaps [2, 3, 4], PhC

waveguides [5] and cavities [6], as well as boundary value problems for finite PhCs [7, 8, 9, 10] and general PhC devices [11, 12].

2. Computing DtN maps

Mathematical formulations for electro-magnetic waves including light, can be classified as two-dimensional (2D), quasi-2D and full three-dimensional (3D). The simplest problems are posed as 2D problems, where the structure is described by a z-independent refractive index function $n = n(\mathbf{x})$ for $\mathbf{x} = (x, y)$ and the waves do not propagate in the z direction, so that the z-derivative of both electric and magnetic fields are zero. In that case, we need to consider two different polarizations. For the E-polarization, we have the Helmholtz equation

$$\partial_x^2 u + \partial_y^2 u + k_0^2 n^2(\mathbf{x}) u = 0, \tag{1}$$

where u is associated with the z component (the only non-zero component) of the electric field, $k_0 = \omega/c$ is the wavelength in vacuum, ω is the angular frequency and c is the speed of light in vacuum. This is a frequency domain formulation, where the z component of the electric field is actually the real part of $ue^{-i\omega t}$. For the H-polarization, we have a slightly different governing equation for the z component of the magnetic field. In the quasi-2D case, the refractive index is still z-invariant, but we allow the waves to propagate in the z direction in the simple form of $e^{i\beta z}$, where β is either given or an unknown to be determined. In that case, we still need to solve 2D problems, but it is necessary to work on two components of the electric-magnetic fields together. For example, we can simplify the Maxwell's equations to a system of two equations for the z-components of both electric and magnetic fields. The z-derivatives in the equations are replaced by $i\beta$, therefore these equations are still solved in the xy plane. In full 3D case, the refractive index is a function of all three variables.

PhC structures and devices have only a small number of distinct unit cells. We calculate the DtN maps of the unit cells and use them for further computations. Two-dimensional PhCs are typically composed of circular cylinders in a square or triangular lattice. The cylinders are either dielectric rods or air holes. Outside the cylinders, we have a homogeneous medium which could be just air if the cylinders are dielectric rods. Typically, we choose a unit cell Ω to include the whole cylinder inside. A number of different methods are available to find the DtN map of Ω. The simplest method is based on special solutions in Ω and collocation on the boundary. Let us consider the E polarization. First, we find K special solutions ϕ_k ($k = 1, 2, ..., K$) for the governing equation (1), and assume that the general solution in Ω is a linear combinations of these special solutions:

$$u(\mathbf{x}) \approx \sum_{k=1}^{K} c_k \phi_k(\mathbf{x}), \quad \mathbf{x} \in \Omega. \tag{2}$$

Next, we choose K points on $\partial\Omega$, that is $\mathbf{x}_j$ for $j = 1, 2, ..., K$, and also choose the associate unit vectors $\nu_j = \nu(\mathbf{x}_j)$, then evaluate $\phi_k(\mathbf{x}_j)$ and $\partial_{\nu_j}\phi_k(\mathbf{x}_j)$ for all j and k. Finally, the DtN map of Ω is approximated by the matrix $\Lambda = BA^{-1}$, where A and B are $K \times K$ matrices whose (j, k) entries are $\phi_k(\mathbf{x}_j)$ and $\partial_{\nu_j}\phi_k(\mathbf{x}_j)$, respectively. For circular cylinders, the special solutions are available analytically. They are the cylindrical waves as in the Fourier-Bessel expansion [7]. For more general cylinders,

we can use a boundary integral equation method to construct the special solutions [4]. If the unit cell Ω is a union of a few sub-cells, we can calculate the DtN map of Ω by merging the DtN maps of the sub-cells [8]. If the unit cell Ω contains a few randomly placed and possibly different circular cylinders, we can use the multipole method to find the special solutions [9]. Recently, we have constructed DtN maps for anisotropic media, for quasi-2D cases and for photonic crystal slabs which are 3D structures with 2D periodicity.

3. Application to eigenvalue problems

The DtN maps have been used to solve a number of eigenvalue problems for PhCs. For an infinite and perfectly periodic PhC, the fundamental problem is to calculate its band structures. Consider the E polarization again, we now assume $n(\mathbf{x})$ is periodic in two different directions with two possibly different periods. For such a periodic structure, we consider Bloch wave solutions given by

$$u = e^{i(\alpha x+\beta y)}\Phi(\mathbf{x}), \tag{3}$$

where Φ follows the same periodicity as $n(\mathbf{x})$, (α, β) is the Bloch wave vector. Such a solution does not exist for all frequency. They only exist for a discrete sequence of frequencies given by

$$\omega = \omega_l(\alpha, \beta), \quad l = 1, 2, ... \tag{4}$$

These relations between the wave vector and the frequency are the dispersion relations. They reveal the band structure of the PhC. If a frequency ω does not satisfy a dispersion relation for any real (α, β) and any l, then it is in a bandgap. The standard band structure problem is an eigenvalue problem formulated on Ω with quasi-periodic boundary conditions (since α and β are assumed to be real and given), where (1) is the governing equation (for the 2D E-polarization case) and ω^2 (or k_0^2) is the eigenvalue [1]. Using DtN maps of the unit cell, we have re-formulated the eigenvalue problem on the boundary of Ω [2, 3, 4]. Our approach is to solve β (or α) assuming ω and α (or β) are given. Since only the boundary is involved, we obtain an eigenvalue problem for much smaller matrices. We also note that when the medium is dispersive, i.e., the refractive index n depends on frequency ω, the standard formulation using ω^2 as the eigenvalue becomes nonlinear and more difficult to solve. In our formulation based on DtN maps, ω is given and the eigenvalue is related to α or β, so the problem remains linear even for dispersive media.

When a line defect is introduced in an otherwise perfectly periodic PhC, for example by removing a row of rods or filling a row of holes, we obtain a PhC waveguide. Assuming that the waveguide axis is parallel to the x-axis, the refractive index $n(\mathbf{x})$ is now only periodic in x. For such a line defect waveguide, we seek propagating modes for frequency in a bandgap. Such a propagating mode is again a Bloch mode given by

$$u(\mathbf{x}) = e^{i\alpha x}\Phi(\mathbf{x}), \tag{5}$$

where α is real, Φ is periodic in x and $\Phi \to 0$ as $y \to \pm\infty$. Such a solution only exist when ω and α satisfy a relation (the dispersion relation). Notice that the problem for PhC waveguide is very similar to the problem of band structure. The difference is that for a PhC waveguide, we must replace the unit cell of the original PhC by the supercell which cover one period in the x direction and for $-\infty < y < \infty$. Fortunately,

since the frequency is in a bandgap (of the original PhC without the line defect), the solution decays to zero as $|y|$ is increased. Therefore, we can truncate y to a finite interval with simple boundary conditions, such as $u = 0$. If we keep m unit cells in the y direction, the standard eigenvalue problem is then formulated on a truncated supercell covering m unit cells. Using our DtN maps, we have re-formulated the eigenvalue problem on the boundary of the supercell [5]. Notice that we need the DtN map of the supercell. This is easy to obtain once the DtN maps of the (regular and defect) unit cells are calculated.

A point defect in a PhC creates a microcavity which could trap light around it, if the frequency is in a bandgap. However, this is true only for some special frequencies in bandgaps. Mathematically, it is an eigenvalue problem given by the Helmholtz equation (1) in the entire xy plane with the boundary condition $u \to 0$ as $r = \sqrt{x^2 + y^2} \to \infty$, and the eigenvalue is ω^2. Since the frequency is in a bandgap and the eigenfunction u decays as r is increase, we can truncate the domain and solve the eigenvalue problem numerically. The truncated domain is still much larger than a single unit cell, therefore, the matrix is typically very large. Furthermore, the eigenvalue of the cavity mode is an interior eigenvalue of the eigenvalue problem on the truncated domain, since there are many other eigenvalues outside the bandgap. Unfortunately, an interior eigenvalue of a large matrix is very difficult to calculate by existing numerical techniques. Using the DtN maps, we have developed an accurate and efficient method for computing defect modes [6]. We find the frequency of the defect mode iteratively from the condition that a small matrix is singular. Since the method is iterative, we need to find that small matrix for a given ω. We proceed with a truncation of the xy plane as in other methods. With the help of DtN maps for the regular and defect unit cells, we establish a system of homogeneous equations for u on all edges of the unit cells. The system is in fact sparse, since the equation for an edge is obtained from the DtN maps of the two neighboring unit cells, thus it involves only the edges of these two cells. Using Gaussian elimination, we can reduce the linear system on all edges in the truncated domain to a small linear system on a single edge near the defect. This is a homogeneous system which must have a singular coefficient matrix when ω is the frequency of the defect mode.

Using DtN maps, we have also analyzed leaky waveguides and leaky cavities. Instead of a line defect in an infinite PhC, if the PhC crystal in each side of the line defect is finite, the waveguide could be leaky, i.e., α in (5) is complex. The imaginary part of α should be positive, then, as the mode propagate towards $x = +\infty$, its amplitude decays exponentially. Similarly, if a cavity is surrounded by a finite PhC photonic crystal or close to a PhC waveguide, the eigenvalue problem (1) may have no solution that decays at infinity. In that case, we seek a solution with complex ω such that it decreases in time (based on our assumed time dependence $e^{-i\omega t}$). For a leaky waveguide mode, the field diverges in the transverse direction (i.e. the y direction). Similarly, the field of a leaky cavity mode diverges at infinity.

4. Application to boundary value problems

Using DtN maps, we have developed some efficient methods for solving boundary values problems of PhC structures. A simple boundary value problem is associated with the scattering a plane wave on a PhC which is finite in one direction and still infinite and periodic in the other direction. For 2D PhCs, this is the diffraction of

finite number of arrays of cylinders, where each array is infinite and periodic. If the structure is periodic in x with period a and finite in y given by $0 < y < D$. We can formulated the problem on the rectangle S given by $0 < x < a$ and $0 < y < D$. If an incident plane wave is specified for $y > D$, we have rigorous boundary conditions at $y = 0$ and $y = D$ and quasi-periodic conditions at $x = 0$ and $x = a$. The problem can be solved on S directly. However, if we divide S into a number of unit cells and calculate the DtN maps of the unit cells, we can reduce the problem to the edges of the unit cells in S and obtain a very efficient method [7, 8, 9, 10]. Similar methods have also been developed for quasi-2D problems using two coupled field components, and for 3D structures including crossed arrays of cylinders (the woodpile structure) and PhC slabs.

A general linear and passive PhC device can be regarded as an assembly of cavities and waveguides (point and line defects) in a finite domain connected to infinity by a few PhC waveguides (ports). We have developed DtN map method for analyzing general 2D PhC devices [11]. If the domain is properly truncated, we can establish a sparse linear system on the edges of the unit cells using DtN maps, just like the equations in [6]. However, there are PhC waveguides extending to infinity. These waveguides cannot be terminated with a simple boundary condition, since they allow incoming and outgoing waves without damping. Using the DtN maps, we have developed an efficient method to set up proper boundary conditions for terminating waveguides. The first step is to calculate the DtN map of the supercell for the waveguide. Based on that, we calculate the Bloch modes of the waveguide given as in (5) but for both real and complex α. Using the Bloch modes, we can separate incoming and outgoing waves and finally obtain a rigorous boundary conditions. With these boundary conditions, we can analyze a PhC device in a relatively small domain, then solve a linear system on edges of the unit cells in the truncated domain. If the truncated domain is still large, we can use additional techniques to speed up the computation [12].

5. Conclusion

Photonic crystals have promising applications in future integrated circuits based on lightwaves. With point and line defects, various PhC components and devices have been developed. The design and optimization of these structure require efficient numerical methods. Due to the existence of many identical unit cells in a typical PhC structure, it is advantageous to first calculate the DtN maps of the unit cells and then analyze the structure on the edges of the unit cells (avoiding the interiors of the unit cells completely). From the work reviewed in this paper, it is clear that the DtN map approach is efficient for many different computation problems associated with PhCs.

References

[1] J. D. Joannopoulos, R. D. Meade and J. N. Winn, *Photonic Crystals: Molding the Flow of Light*, Princeton University Press, Princeton, NJ. 1995.

[2] J. Yuan and Y. Y. Lu, "Photonic bandgap calculations using Dirichlet-to-Neumann maps," *Journal of the Optical Society of America A,* Vol. 23, pp. 3217-3222, Dec. 2006.

[3] J. Yuan and Y. Y. Lu, "Computing photonic band structures by Dirichlet-to-Neumann maps: The triangular lattice," *Optics Communications*, Vol. 273, pp. 114-120, May 2007.

[4] J. Yuan, Y. Y. Lu and X. Antoine, "Modeling photonic crystals by boundary integral equations and Dirichlet-to-Neumann maps," *Journal of Computational Physics*, Vol. 227, No. 9, pp. 4617-3629, April 2008.
[5] Y. Huang, Y. Y. Lu and S. Li, "Analyzing photonic crystal waveguides by Dirichlet-to-Neumann maps," *Journal of the Optical Society of America B*, Vol. 24, No. 11, pp. 2860-2867, Nov. 2007.
[6] S. Li and Y. Y. Lu, "Computing photonic crystal defect modes by Dirichlet-to-Neumann maps," *Optics Express*, Vol. 15, No. 22, pp. 14454-14466, Oct. 29, 2007.
[7] Y. Huang and Y. Y. Lu, "Scattering from periodic arrays of cylinders by Dirichlet-to-Neumann maps," *Journal of Lightwave Technology,* Vol. 24, pp. 3448-3453, Sept. 2006.
[8] Y. Huang and Y. Y. Lu, "Modeling photonic crystals with complex unit cells by Dirichlet-to-Neumann maps," *Journal of Computational Mathematics*, Vol. 25, No. 3, pp. 337-349, May 2007.
[9] S. Li and Y. Y. Lu, "Multipole Dirichlet-to-Neumann Map method for photonic crystals with complex unit cells," *Journal of the Optical Society of America A*, Vol. 24, pp. 2438-2442, Aug. 2007.
[10] Y. Wu and Y. Y. Lu, "Dirichlet-to-Neumann map method for analyzing interpenetrating cylinder arrays in a triangular lattice," *Journal of the Optical Society of America B*, Vol. 25, pp. 1466-1473, No. 9, Sept. 2008.
[11] Z. Hu and Y. Y. Lu, "Efficient analysis of photonic crystal devices by Dirichlet-to-Neumann maps," *Optics Express*, Vol. 16, No. 22, pp. 17383-17399, Oct. 2008.
[12] Z. Hu and Y. Y. Lu, "Improved Dirichlet-to-Neumann map method for modeling extended photonic crystal devices," submitted for publication.

Department of Mathematics, City University of Hong Kong, Kowloon, Hong Kong
E-mail address: mayylu@cityu.edu.hk