Engineering Analysis with Boundary Elements 68 (2016) 42–53

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

Periodic band structure calculation by the Sakurai–Sugiura method with a fast direct solver for the boundary element method with the fast multipole representation

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ARTICLE INFO

Article history:
Received 5 October 2015
Received in revised form
23 March 2016
Accepted 30 March 2016
Available online 9 April 2016

Keywords:
Photonic/Phononic band structure
Periodic problem
Sakurai–Sugiura method
Non-linear eigenvalue problem
Fast direct solver for boundary element method
Fast multipole method

ABSTRACT

In this paper, we present a numerical method for periodic band structure calculation, which is associated with eigenvalue problems for periodic problems, using the boundary element method (BEM). In the BEM, the eigenvalue problems are converted into non-linear eigenvalue problems, which are not tractable with conventional eigensolvers. In the present study, to solve non-linear eigenvalue problems, the block Sakurai–Sugiura (SS) method, which can convert non-linear eigenvalue problems into generalised eigenvalue problems, is utilised. A fast direct solver for the BEM with a fast multipole representation is employed in the algorithm of the block SS method since algebraic equations need to be solved for multiple right-hand sides in the block SS method. We conduct several numerical experiments related to phononic structures to confirm the validity and efficiency of the proposed method. We confirm that the proposed method can calculate the band structure of the phononic structures, and the computational time with the proposed method is less than that with a conventional FEM-based eigensolvers with triangular linear elements even for relatively small problems.

1. Introduction

In the last several decades, periodic structures such as photonic and phononic crystals have attracted considerable attention of researchers and engineers [1]. This is because these materials have complete bandgaps for waves. A complete bandgap is defined as a frequency range in which waves cannot propagate in any direction. A periodic dielectric material which has bandgaps for an electromagnetic wave (including light) is called a photonic crystal and its elastic counterpart is called a phononic crystal or structure. These materials are expected to be used in the next generation of wave devices, such as lasers, waveguides, and slow light in the field of optics and acoustic filters, noise controlling devices, and transducers in the field of mechanics. To realise these technologies, it is important to develop a fast and accurate numerical solver for bandgap calculations.

Several numerical methods for bandgap calculations have been proposed. As classical methods, we can mention plane wave expansion (PWE) [2,3] and the multiple scattering theory (MST) [4,5]. The applicability of these methods is limited to problems with simple geometry. As general methods for bandgap calculations, although the finite difference in time domain (FDTD) method and the finite element method (FEM) are widely used, the applicability of these methods may not be sufficient for realistic engineering problems in some cases. The FDTD requires the discretisation of the whole domain, which makes it difficult to apply this method to large-scale photonic/phononic simulations, particularly in three-dimensional domain. Further, since FDTD is a method to solve the wave equation in the time domain, we need to calculate wave propagation for sufficiently long period of time for waves containing various frequencies, and convert the obtained wave distribution into the spectrum domain, which may be time consuming, particularly for three-dimensional problems with a complex geometry. Although the FEM can directly solve the eigenvalue problems in the frequency domain, it still suffers from domain discretisation. It is known that, when *hp*-FEM is used to calculate eigenvalues for partial differential equations (PDEs), the eigenvalues converge exponentially as the degree of freedom (DoF) increases [6]. Although the exponential convergence is attractive, *hp*-FEM is, to the knowledge of the authors, not necessarily widely used for band structure calculation. This is partly because the implementation of the *hp*-FEM is relatively complicated, and the mesh discretisation cost is expensive for complicated geometry.

As a possible alternative for numerical bandgap calculations, we can mention the boundary element method (BEM). We, however, encounter non-linear eigenvalue problems which are not

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http://dx.doi.org/10.1016/j.enganabound.2016.03.018
0955-7997/

tractable with conventional eigensolvers when we naively employ the BEM to reformulate the eigenvalue problems related to periodic problems. Irrespective of its difficulty to deal with the non-linear eigenvalue problem, some researchers have proposed bandgap calculations with the BEM [7–10]. These methods are classified into the following two categories:

- Consider the frequency ω as a given parameter and the Bloch wave vector k as an eigenvalue.
- Consider the Bloch wave vector k as a given parameter and the frequency ω as an eigenvalue.

The former gives a generalised (resp. quadratic) eigenvalue problem for a square (resp. triangular) lattice, while the latter gives a non-linear eigenvalue problem [7]. Li et al. [7,8] used the former approach, and successfully solved photonic/phononic band structures by relaxing the periodic boundary condition to ensure numerical stability. Yuan et al. [9] are also considered as the former approach, in which a Dirichlet-to-Neumann map is utilised. As an example of the latter method, Barnett and Greengard [10] presented an efficient evaluation of the Green function, which satisfies the periodic boundary condition, and its application to bandgap calculations. Since they focused on the evaluation of the periodic Green function, they simply plotted the smallest singular value of the relevant matrix to find the eigenvalue. Thus, there are few studies on an effective numerical method to solve the non-linear eigenvalue problem stemming from the latter approach.

Recently, some promising solvers for non-linear eigenvalue problems are developed; Sakurai–Sugiura (SS) method [11,12], non-linear Arnoldi method [13] and the infinite Arnoldi method [14]. Among them, the SS method shall be used in this paper. Sakurai and Sugiura originally proposed the SS method to find certain eigenvalues of a generalised eigenvalue problem that lie in a given domain of the complex plane [11], and Asakura et al. pointed out the possibility that the SS method can solve a non-linear eigenvalue problem [12]. Since its development, applications of the SS method are rapidly enhanced. The SS method is, thus far, applied to the calculations of the core-excited state of formaldehyde [15], eigenvalue problems in lattice quantum chromodynamics (QCD) [16], eigenvalue problems in 2D and 3D Helmholtz' equations [17,18], eigenvalue problems related waveguides [19], etc. Also, as a similar method to the SS method, we can mention the method by Beyn [20]. In our previous paper [21], we have attempted to apply the SS method to calculate the bandgap for a phononic structure in 2D. Since the conventional BEM without any acceleration technique is combined with the SS method in [21], we have calculated bandgaps for a simple phononic structure which has a circular scatterer in the unit cell. In order to deal with a more complex geometry, in this paper, we present a combination of an accelerated BEM with the SS method.

In the algorithm of the SS method, when multiple eigenvalues are concerned, we need to solve algebraic equations with multiple right-hand sides (block SS method). Because of the multiple right-hand sides, the use of the widely used fast multipole boundary element method (FMBEM) [22,23], which involves iterative solvers for algebraic equations, may not accelerate the eigensolver. In such a case, it is preferable to use a direct solver rather than an iterative solver to solve the algebraic equations. Thus far, some fast direct solvers, in which algebraic equations of size N obtained as a discretised boundary integral equation can be solved by a direct solver with an $O(N\log^{\alpha}N)$, $(\alpha=0,1,2)$ computational complexity, have been proposed [24,25]. In this study, we utilise a direct solver for the BEM with a fast multipole representation [26], which is henceforth denoted as "direct FMM". Although the direct FMM might not achieve $O(N\log^{\alpha}N)$ complexity for large N, it is relatively easy to implement and is efficient for moderately sized problems. Thus, our main focus in this paper is to accelerate bandgap calculations with the BEM and the SS method for 2D photonic/phononic crystals with a relatively complex geometry which can be modelled with moderate N.

The rest of the paper is organised as follows: After eigenvalue problems related to photonic/phononic crystals and its reformulation with the boundary integral equation are stated in Sections 2.1 and 2.2, respectively, the formulation of the SS method is reviewed in Section 2.3. In Sections 2.4 and 2.5, we present the formulation of the direct FMM and its extension for periodic problems, respectively. In Section 3, we show some numerical examples to show the validity and the efficiency of the proposed method.

Although we focus on orthotropic periodic problems in this paper, other general periodic problems can be appropriately formulated with minor modifications.

2. Formulation

2.1. Statement of the eigenvalue problem associated with periodic structures

We consider a doubly orthotropic periodic array of scatterers in elastic matrix Ω embedded in the unit cell $U:=\{x|0<x_i<L_i,\ i=1,2\}$, where L_i denotes the period along the x_i-axis (Fig. 1). Let $u(x)$ be an out-of-plane time harmonic displacement satisfying the following Helmholtz equation:

$$\nabla^2 u(x)+\omega^2\frac{\rho}{\mu}u(x)=0\quad x\in\Omega, \tag{1}$$

where ρ, μ and ω denote the density, the shear modulus and the angular frequency, respectively. We are interested in finding ω with which a non-trivial function u satisfies the Helmholtz equation (1) along with the following homogeneous boundary conditions:

$$u(x)=0\quad x\in\Gamma_u, \tag{2}$$

$$q(x):=\frac{\partial u(x)}{\partial n}=0\quad x\in\Gamma_q, \tag{3}$$

and the following quasi-periodic boundary conditions:

$$u(x+a_i)=u(x)\exp(\mathrm{i}k\cdot a_i)\quad x\in\Gamma_{\mathrm{I}}, \tag{4}$$

$$\frac{\partial u}{\partial x_i}(x+a_i)=\frac{\partial u}{\partial x_i}(x)\exp(\mathrm{i}k\cdot a_i)\quad x\in\Gamma_{\mathrm{I}}, \tag{5}$$

where $\Gamma_u\subset\Gamma_{\mathrm{B}}:=\partial\Omega$ and $\Gamma_q:=\Gamma_{\mathrm{B}}\backslash\overline{\Gamma_u}$ denote Dirichlet and the Neumann boundary, respectively. Γ_{I} represents a part of the boundary of U defined as $\Gamma_{\mathrm{I}}:=\cup_{i=1,2}\Gamma_{\mathrm{I}i}$, $\Gamma_{\mathrm{I}i}=\{x|0<x_{3-i}<L_{3-i},\ x_i=0,\ i=1,2\}$. We

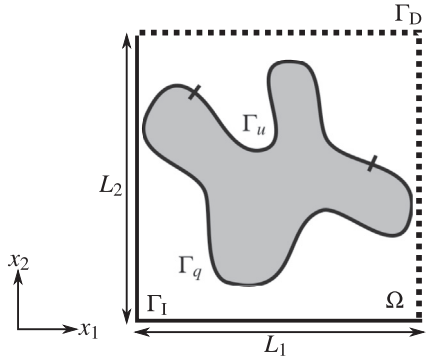

Fig. 1. Periodic problem.