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Variational methods for phononic calculations

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H I G H L I G H T S

- Convergence properties of three variational principles for phononics are studied.
- Convergence found to depend upon smoothness of material properties.
- Mixed variational method shows faster convergence than traditional Rayleigh quotient.

A R T I C L E I N F O

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Three fundamental variational principles used for solving elastodynamic eigenvalue problems are studied within the context of elastic wave propagation in periodic composites (phononics). We study the convergence of the eigenvalue problems resulting from the displacement Rayleigh quotient, the stress Rayleigh quotient and the mixed quotient. The convergence rates of the three quotients are found to be related to the continuity and differentiability of the density and compliance variation over the unit cell. In general, the mixed quotient converges faster than both the displacement Rayleigh and the stress Rayleigh quotients, however, there exist special cases where either the displacement Rayleigh or the stress Rayleigh quotient shows the exact same convergence as the mixed-method. We show that all methods converge faster for smoother material property variations, but when density variation is rough, the difference between the mixed quotient and stress Rayleigh quotient is higher and similarly, when compliance variation is rough, the difference between the mixed quotient and displacement Rayleigh quotient is higher. Since eigenvalue problems such as those considered in this paper tend to be highly computationally intensive, it is expected that these results will lead to fast and efficient algorithms in the areas of phononics and photonics.

1. Introduction

The periodic modulation of stress wave existing in periodic composites results in exotic dynamic response. The phononic band-structure [1] induced by the periodic modulation of stress waves has close similarities with areas like electronic band theory [2] and photonics [3]. The rich wave-physics resulting from the periodic modulations offers potential for novel applications such as refractive acoustic devices [4], ultrasound tunneling [5], waveguiding [6], reversed Doppler effect [7], sound focusing [8], hypersonic control [9], negative refraction [10], gradient-index refraction [11], etc. The first step in realizing these applications is to calculate the phononic band-structure. Additionally, some research areas such as phononic band-structure optimization [12–16] and inverse problems in dynamic homogenization [17] depend heavily on the speed, efficiency, accuracy and versatility of the band-structure calculating algorithm. There exist several techniques

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by which band-structures of photonic and phononic composites can be calculated. The plane wave expansion method (PWE) [3,18,19] is easy to implement but converges slowly when material properties show large contrast. The multiple scattering method [20,21] can precisely predict the band structure, but is subject to geometry limitations. The finite element method (FEM) [22–25] is derived from variational principles and it is widely used for computing phononic bandstructures of various geometries. Hussein and Hulbert [25] have presented a mixed finite element approach based on the variation of displacement and strain field, which shares the same mathematical background (Hu–Washizu variational theorem) as the methods presented in this paper. Some other methods are the finite difference time domain method (FDTD) [26,27] and secondary expansions such as the reduced Bloch mode expansion [28] method, etc.

Convergence rates of three variational principles, the displacement Rayleigh quotient, where the displacement field is varied, the stress Rayleigh quotient, where the stress field is varied, and the mixed quotient [29–31,17], where both the displacement and stress fields are varied, are considered in this paper. In addition, we also compare the convergence rates of the variational methods with the most popular band structure algorithms (PWE and displacement based FEM). The mixed quotient was proposed by Nemat-Nasser [29] in 1972, which was derived from the works of Hellinger [32], Prange [33], Reissner [34,35], Hu [36], Washizu [37]. Nemat-Nasser [30] showed that when compliance is constant, the mixed quotient reduces to the displacement Rayleigh quotient and when density is constant, the mixed quotient reduces to the stress Rayleigh quotient. Babuska and Osborn [38] related the convergence behavior of the three variational principles to the smoothness of the compliance and density functions and showed that the mixed quotient, in general, converges faster than the other two methods. Due to its excellent accuracy and efficiency, the mixed variation principle has been recently applied to the study of wave refraction in periodic elastic composites [39,40].

In this paper, the three variational principles which solve the phononic eigenvalue problems are presented in Section 2. The algorithms derived from the variational principles are suitable for applications to arbitrary unit cells. We present the detailed formulation of the eigenvalue problems and their convergence behavior under different compliance and density distribution for 1-D and 2-D periodic composites. In our calculation we consider the effects of different function continuity and differentiability conditions of compliance and density on the convergence rates of the three formulations.

2. Statement of the problem

Phononic computations seek to evaluate the essential properties of sound/stress waves traveling in periodic structures. These properties include the phononic band-structure evaluated along the boundary of the Irreducible Brillouin zone (IBZ) of 1-, 2-, and 3-D composites, their equi-frequency contours, and the associated density of states. However, all these properties emerge from the solution of the fundamental eigenvalue problem which is associated with the elastodynamics of periodic structures. In the following subsections we define the essential properties of the periodic domain under consideration, eigenvalue problem associated with wave propagation in this periodic domain, and the variational methods which can be employed for its solution.

2.1. Periodic domain

In the following treatment repeated Latin indices mean summation, whereas, repeated Greek indices do not. Consider a general 3-dimensional periodic composite. The unit cell of the periodic composite is denoted by Ω and is characterized by 3 base vectors $\mathbf{h}^i,\ i = 1, 2, 3$. Any point within the unit cell can be uniquely specified by the vector $\mathbf{x} = H_i\mathbf{h}^i$ where $0 \le H_i \le 1,\ \forall i$. The same point can also be specified in the orthogonal basis as $\mathbf{x} = x_i\mathbf{e}^i$. The reciprocal base vectors of the unit cell are given by:

$$\mathbf{q}^1 = 2\pi \frac{\mathbf{h}^2 \times \mathbf{h}^3}{\mathbf{h}^1 \cdot (\mathbf{h}^2 \times \mathbf{h}^3)}; \qquad \mathbf{q}^2 = 2\pi \frac{\mathbf{h}^3 \times \mathbf{h}^1}{\mathbf{h}^2 \cdot (\mathbf{h}^3 \times \mathbf{h}^1)}; \qquad \mathbf{q}^3 = 2\pi \frac{\mathbf{h}^1 \times \mathbf{h}^2}{\mathbf{h}^3 \cdot (\mathbf{h}^1 \times \mathbf{h}^2)} \tag{1}$$

such that $\mathbf{q}^i \cdot \mathbf{h}^j = 2\pi\delta_{ij}$. Fig. 1 shows the schematic of a 2-D unit cell, indicating the unit cell basis vectors, the reciprocal basis vectors and the orthogonal basis vectors. The composite is characterized by a spatially varying stiffness tensor, $C_{jkmn}(\mathbf{x})$, and density, $\rho(\mathbf{x})$, which satisfy the following periodicity conditions:

$$C_{jkmn}(\mathbf{x} + n_i\mathbf{h}^i) = C_{jkmn}(\mathbf{x}); \qquad \rho(\mathbf{x} + n_i\mathbf{h}^i) = \rho(\mathbf{x}) \tag{2}$$

where n_i ($i = 1, 2, 3$) are integers. For wave propagation in such a periodic composite the wave vector is given as $\mathbf{k} = Q_i\mathbf{q}^i$ where $0 \le Q_i \le 1,\ \forall i$.

2.2. Field equations and boundary conditions

For harmonic elastodynamic problems the equation of motion at any point $\mathbf{x}$ in Ω is given by

$$\sigma_{jk,k} = -\lambda\rho u_j \tag{3}$$

where $\lambda = \omega^2$, and $\boldsymbol{\sigma} \exp[-i\omega t]$, $\mathbf{u} \exp[-i\omega t]$ are the space and time dependent stress tensor and displacement vector respectively. The stress tensor is related to the strain tensor through the elasticity tensor, $\sigma_{jk} = C_{jkmn}\varepsilon_{mn}$, and the strain