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A postprocessing method based on high-resolution spectral estimation for FDTD calculation of phononic band structures

Xiao-Xing Su [a,*], Jian-Bao Li [b], Yue-Sheng Wang [b]

[a] School of Electronic and Information Engineering, Beijing Jiaotong University, Beijing 100044, China
[b] Institute of Engineering Mechanics, Beijing Jiaotong University, Beijing 100044, China

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ABSTRACT

If the energy bands of a phononic crystal are calculated by the finite difference time domain (FDTD) method combined with the fast Fourier transform (FFT), good estimation of the eigenfrequencies can only be ensured by the postprocessing of sufficiently long time series generated by a large number of FDTD iterations. In this paper, a postprocessing method based on the high-resolution spectral estimation via the Yule–Walker method is proposed to overcome this difficulty. Numerical simulation results for three-dimensional acoustic and two-dimensional elastic systems show that, compared with the classic FFT-based postprocessing method, the proposed method can give much better estimation of the eigenfrequencies when the FDTD is run with relatively few iterations.

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1. Introduction

Phononic crystals (PCs) [1] are a kind of composite materials which are formed by periodic variation of the acoustic properties (i.e., mass density and elastic moduli) of the materials. The most fundamental and attractive property of PCs is the possibility of having complete band gaps, the frequency intervals where the propagation of acoustic waves (AWs) or elastic waves (EWs) is fully forbidden in all directions. Therefore, the theoretical study of PCs is focused on the energy band calculation. The numerical methods developed for phononic energy band calculation include the plane wave expansion (PWE) method [2,3], multiple scattering theory (MST) [4,5], the wavelet method [6,7], the finite difference time domain (FDTD) method [8–15] and the finite element method (FEM) [16,17], etc. Among them, the FDTD method has some noticeable advantages, such as its ability to deal with solid/liquid systems [8–11], its suitability to tackle arbitrarily shaped scatterers [12,13] , its good convergence property [8,14] and its easy and efficient parallel implementation [14].

Unlike the frequency domain methods, the FDTD calculation is performed by iterations in the time domain directly, and thus such high-complexity operations as the inversion of matrices can be avoided. However, to obtain the energy bands of a PC by using the FDTD method, a postprocessing method must be applied to the FDTD time series (FDTD-TS), i.e. the discrete time series of one field variable on an observing point computed by FDTD at each iteration. The postprocessing method is based on a spectral analysis algorithm which the fast Fourier transform (FFT) usually serves as for its efficiency and robustness. But the frequency estimation accuracy of FFT is limited by its frequency resolution which is given by

$$\Delta f = \frac{1}{N\Delta t}, \tag{1}$$

where N is the length of the considered time series; and Δt is the time step. Moreover, to ensure the numerical stability [19] of FDTD iterations, the FDTD-TS is so oversampled that its time step is far less than the time interval in which the wave transmits through a unit cell of the PC. Thus, in order to improve the accuracy of the FFT-based postprocessing, a large number of FDTD iterations are often needed to generate sufficiently long FDTD-TS. For example, the numbers of FDTD iterations are at least 100,000 in the simulations reported in [8] and [14]. However, when the computation load of each FDTD iteration is relatively big, much computation time is needed to run so many iterations. A big computation load may occur in the simulations of three-dimensional (3D) systems or systems with high wave impedance ratios between scatterers and the host. In the latter case, the big computation load is caused by a dense spatial mesh which is used for good convergence of the results.

Improvement of the frequency resolution of the spectral estimation with relatively short time series is an intensely discussed topic in modern signal processing. And the high-resolution spectral estimation (HRSE) methods [18] based on

* Corresponding author. Tel.: +86 10 51684017; fax: +86 10 51683625.
E-mail address: xxsu@bjtu.edu.cn (X.-X. Su).

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parametric modeling have attracted the most attention among others. But the efficiency of the HRSE methods is often relatively low if compared with the classic algorithm FFT. Even so, the HRSE methods can still be considered to improve the performance of the spectral analysis of relatively short FDTD-TS, under the precondition that

$$T_{\mathrm{FDTD}} \gg T_{\mathrm{Post}}, \tag{2}$$

where T_{FDTD} is the time spent on all of the FDTD iterations; and T_{Post} is the time spent on the postprocessing. The combination of the FDTD and HRSE has been receiving a certain degree of attention in the field of computational electromagnetic [19–22]. In the simulations of high-Q-valued electromagnetic devices, the field distribution cannot become stable until many FDTD iterations are run, but the HRSE methods can reduce the number of iterations by estimating the frequency response of the devices accurately with relatively short FDTD-TS. In this paper, a postprocessing method based on HRSE via the Yule–Walker (YW) method [18] for FDTD calculation of phononic energy bands is proposed by the authors. The aim is to reduce the number of FDTD iterations by estimating the eigenfrequencies of PCs accurately with relatively short FDTD-TS, under the circumstance of 3D systems or systems with high acoustic impedance ratios. For these systems, a big computation load of each FDTD iteration is necessary and thus the precondition (2) is satisfied.

2. General idea of FDTD calculation of phononic energy bands

The equations for a linear AW in fluids and a linear EW in solids are, respectively, as follows:

AW equations

$$\frac{\partial p(\mathrm{r},t)}{\partial t} = -\frac{1}{\kappa(\mathrm{r})}\nabla \mathrm{v}(\mathrm{r},t), \tag{3}$$

$$\frac{\partial \mathrm{v}(\mathrm{r},t)}{\partial t} = -\frac{1}{\rho(\mathrm{r})}\nabla p(\mathrm{r},t). \tag{4}$$

EW equations

$$\rho(\mathrm{r})\frac{\partial \mathrm{v}(\mathrm{r},t)}{\partial t} = \nabla \boldsymbol{\theta}(\mathrm{r},t), \tag{5}$$

$$\frac{\partial \boldsymbol{\theta}(\mathbf{r},t)}{\partial t} = \mathbb{C}(\mathbf{r}) : \nabla \mathbf{v}(\mathbf{r},t). \tag{6}$$

In Eqs. (3)–(6), p is the acoustic pressure; $\mathbf{v}$ is the velocity vector; ρ is density; and κ is compressibility. In Eqs. (5) and (6), $\boldsymbol{\theta}$ and $\mathbf{C}$ are the stress and elasticity tensors, respectively. For an isotropic medium we have $C_{ijkl}=\lambda\delta_{ij}\delta_{kl}+\mu(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$, where C_{ijkl} denotes the components of the tensor $\mathbf{C}$; λ and μ are Lamé constants. In Eq. (6) the symbol ":" denotes the operation of double dot-product. Based on the Bloch theorem, the wave fields in a periodic medium should take the following form:

$$w(\mathrm{r},t) = W(\mathrm{r},t)e^{j\mathbf{k}\mathrm{r}}, \tag{7}$$

where $j=\sqrt{-1}$, $\mathbf{k}$ is the Bloch wave vector; w denotes an arbitrary field variable (p, $\mathbf{v}$ or $\boldsymbol{\theta}$) in Eqs. (3)–(6); and W is the spatial periodic function with the same periodicity as the crystal lattice.

The FDTD methods used in this paper are based on the AW Eqs. (3), (4) or the EW Eqs. (5), (6) and the Bloch boundary condition (7). To obtain the discretized forms (i.e. difference equations) of the AW or EW equations, the components of the field variables are sampled at integral or half-integral spatial grid-points and time steps in a staggered manner; and the derivatives of the field variables to spatial coordinate and time are approximated by the second-order center difference. For the details of the discretization process, we refer to [8,14] or [15]. For band structure calculation of perfect PCs, the calculation area of the FDTD is the unit cell. For any given Bloch wave vector $\mathbf{k}$, the obtained difference equations are solved by iterations in the time domain after a certain initial condition (i.e. the excitation source) is set at the beginning. The FDTD-TS is recorded on each of the observing points which are randomly selected beforehand.

In the postprocessing method, FFT is usually applied to the FDTD-TS corresponding to each observing point to obtain the power spectrum (i.e. the square of the magnitude of the frequency spectrum). Then the obtained power spectra are averaged over all the observing points. The peaks in the averaged power spectrum are identified as the eigenfrequencies of the PC. By using the averaged power spectrum instead of a single power spectrum corresponding to only one observing point, the estimation accuracy of the eigenfrequencies can be improved and the missing of the eigenfrequencies caused by the accidental coincidence of the nodal points of the eigenfunctions with the observing points can be avoided. The commonly used algorithms of detecting peaks from a spectrum include the second-order derivative method and the wavelet method [23]. The simplest second-order derivative method is suitable for use in the case of a high signal-to-noise ratio (SNR). Because the noise in FDTD-TS (mainly induced by digital quantization) can almost be neglected, the second-order derivative method is used to detect peaks from the averaged spectrum of the FDTD-TS in this paper.

3. Postprocessing method based on HRSE

The proposed postprocessing method includes two main steps: preprocessing of FDTD-TS and power spectrum estimation. The details about the two main steps will be given in Sections 3.1 and 3.2, respectively. The preprocessing step is further subdivided into three minor steps: filtering, decimation and normalization. The aim of the preprocessing is to improve the performance of the subsequent spectrum estimation. A summary of the complete method will be given in Section 3.3.

3.1. Preprocessing of FDTD-TS

For the energy band diagram of a PC, we are usually more concerned about the part where the normalized frequency (Ω) is less than a certain value ($\Omega_{\max}$). In this paper, the normalized frequency is defined as $\Omega=fa/c_{\mathrm{B}}$, where f is the frequency; a is the lattice constant; and c_{B} is the transverse or longitudinal wave velocity of the host material. Compared with $\Omega_{\max}$ which is generally less than 3, the FDTD-TS is a highly oversampled time series. Filtering and decimation (FD) are the commonly used operations in the frequency-zooming techniques [24] and the narrow-band high-resolution analysis [25,26] of signals. In the papers [19–22] in computational electromagnetics cited in the introduction, the FD operations were all used to preprocess the FDTD-TS. After the FD operations, the length of the over-sampled time series reduces significantly without loss of frequency resolution. The improvements of the performance of the spectrum estimation caused by the FD operations include: improvement of the frequency resolution, decreasing of the output noise and reduction of the computation load [25].

In the filtering operation, a low-pass filter with the normalized frequency band $[0, \Omega_{\max}]$ can be used because the maximum normalized frequency we still show interest in is $\Omega_{\max}$. According to the Nyquist sampling theorem [24], the sampling frequency used in the following decimation operation should be at least two times the maximum frequency of the filtered FDTD-TS.

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