Structural optimization of phononic crystals

R Adhithya

I. Problem statement

Over the last two decades, phononic crystals have gained much attention, and the theoretical concept of phononic crystals has been developed extensively. The phenomenon of tunable novel effects of PnCs lays a significant foundation for designing phononic crystal materials and structures for effects of interest and potential applications.

The topology optimization problem of phononic crystals can be generally defined as

$$min(f_i(\Sigma)) \qquad i = 1, 2..N \tag{1}$$

s.t.
$$g(\Sigma) \le g_j$$
, $j = 1, 2...M$ (2)

$$\nabla.(\mathbf{C}(\mathbf{x}): \nabla_{s}\mathbf{u}(\mathbf{x})) + \lambda\rho(\mathbf{x})\mathbf{u}(\mathbf{x}) = 0$$

$$\mathbf{u}(\mathbf{x} + \mathbf{h_{i}}) = \mathbf{u}(\mathbf{x})\exp(i\mathbf{k}.\mathbf{h_{i}})$$

$$\sigma(\mathbf{x} + \mathbf{h_{i}}).\mathbf{n}(\mathbf{x} + \mathbf{h_{i}}) = \sigma(\mathbf{x}).\mathbf{n}(\mathbf{x})\exp(i\mathbf{k}.\mathbf{h_{i}})$$
(3)

where $\lambda = \omega^2$.

$$\sigma(\mathbf{x}).\mathbf{n}(\mathbf{x}) = 0 \text{ on } \Gamma_{hole}$$

$$[[\mathbf{u}(\mathbf{x})]] = 0 \text{ on } \Gamma_{mat}$$

$$[[\sigma(\mathbf{x}).\mathbf{n}(\mathbf{x})]] = 0 \text{ on } \Gamma_{mat}$$
(4)

where Σ denotes the topological distribution within the unit cell of the PnCs. $f_i(\Sigma)$ are, respectively, objective functions of the topological distribution that aim to be maximized and minimized. $g(\Sigma)$ are, respectively, the constraint equations.

The first stage is to calculate the band structure of the PnCs for a given design and measure the band gap widths existing in the band structure by solving eq. (3) subject to boundary conditions in eq. (4). The second stage is to mathematically solve the optimization model and address the solution for the current optimization problem explained in eq. (1), eq. (2)[1].

A. Objective functions

Two popular approaches are used to construct the objective function used for optimization. The first way is the difference between two adjacent eigenfrequencies, called the absolute gap width

$$f_1(\Sigma) = \omega_{n+1}(\Sigma; \mathbf{k}) - \omega_n(\Sigma; \mathbf{k}) \tag{5}$$

The second way is use a central frequency as a measure to evaluate the bandg gap around it. This called as the relative band gap width.

$$f_1(\Sigma) = 2 \frac{\min_{\mathbf{k}} : \omega_{n+1}(\Sigma; \mathbf{k}) - \max_{\mathbf{k}} : \omega_n(\Sigma; \mathbf{k})}{\min_{\mathbf{k}} : \omega_{n+1}(\Sigma; \mathbf{k}) + \max_{\mathbf{k}} : \omega_n(\Sigma; \mathbf{k})}$$
(6)

Alternative expressions for eq. (5), and eq. (6) by replacing $\omega_n(\Sigma; \mathbf{k})$ and $\omega_{n+1}(\Sigma; \mathbf{k})$ with their square values, $\omega_n^2(\Sigma; \mathbf{k})$ and $\omega_{n+1}^2(\Sigma; \mathbf{k})$

II. Optimization techniques

There are several works, where gradient-based and gradient-free topology optimization techniques are used to design the band structure for phononic crystals. The gradient-based topology optimization techniques require a relatively small number of function evaluations while the gradient-free techniques require larger number of function evaluations but can be used for multi-objective optimization problems.

A. Gradient-based topology optimization

In gradient-based topology optimization techniques, the initial discrete problems are relaxed by assuming continuous design variables in the interval [0, 1]. The corresponding material properties at points between 0 and 1 can be interpolated by the material properties at 0 and 1. This technique is known as the inverse homogenization or density-based methods. This technique was first applied to band gap design of phononic crystal materials by Sigmund [2] and Sigmund and Jensen [3] through a linear material interpolation scheme. Scheme. In this approach, the prescribed elastic properties in an element are assumed to be defined as

$$A_e(x_e) = (1 - x_e)A_1 + x_e A_2 \tag{7}$$

where subscripts e, 1, and 2 respectively, denote the element number, material phase 1, and material phase 2 and $x_e \in [0, 1]$. Several works based on the above philosophy were conducted. One of the common issues with the above method is the intermediate values of the material properties at the boundary of the interface. The problem is solved using explicit mesh-independent penalization scheme as an extra constraint.[4]. The common optimization techniques used are the method of moving asymptotes (MMA)[5] and bi-directional evolutionary structural optimization (BESO) method [6] along with FEM.

The issue with the density-based methods can also be solved by using methods like level-set method, heaviside projection method and phase-field method to accurately represent the boundary of the interface. The level set method is used in tandem with Interface-enriched Generalized Finite Element Method (IGFEM). The level set-based topology optimization procedure is used in combination with IGFEM in order to find optimized unit cell topologies for band gap maximization without staircased boundaries [7]. The method was used for both 2-D and 3-D phononic crystals as shown in fig. 1 to show promising results. In this work, MMA was used for topology optimization. The topology optimization can only

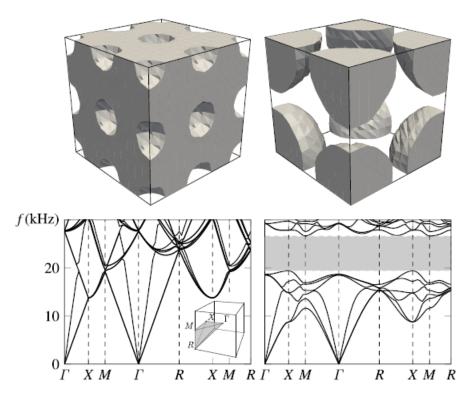


Fig. 1 3-D results of band gap maximization

modify the existing structure and it is seen that there are many local optima to which the optimizer may converge that may not even show a band gap at all. Two suggestions were mentioned as prospective future work directions. The first is to use a method to nucleate inclusions in the design and the second is to use a globally convergence method of moving asymptotes (GCMMA) to avoid oscillations in the objective function due to MMA.

B. Gradient-free topology optimization

Genetic Algorithm (GA) is the most popular approach that has been used for topology optimization of phononic band gaps. Contrary to the gradient-based methods, no material interpolation assumption or complicated sensitivity calculation are required to perform the GA method. A 0–1 integer programming formulation is devised for further optimization solutions.

Several works on using FEM and GA methods to use topology optimization of phononic crystals exist. Hussein et al.[8] conducted the phononic band gap design for 2D PnCs based on the FEM and the GA method. Based on the GA-driven optimization approach, they studied a range of Young's modulus and density ratios for the optimal unit cell designs in the out-of-plane mode. Bilal and Hussein [9],[10] reported a specialized genetic-algorithm-based topology optimization method for maximization of the absolute band gap in 2D solid/void porous PnCs for simultaneous attenuation of out-of-plane and in-plane waves. The common variants of GA used are multi-elitist GA (MEGA) [11], multi-objective GA (MOGA) [12], and non-dominated sorting genetic algorithm (NSGA) [13].

Interest has been taken to use deep learning as they also have the advantage of gradient-free methods of solving multi-objective optimization problems. In one such work, a general architecture of deep learning model, which is composed of two main parts: (1) the encoder (CNN) and (2) the dense layers (ANN) is used fig. 2. The main novelty of the proposed approach relies on the use of non-uniform rational basis spline (NURBS) curves instead of pixels and/or mesh elements to control the shape of the unit cells of phononic crystals [14]

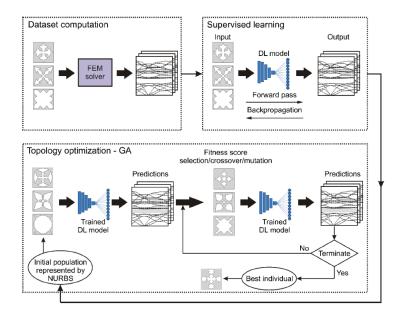


Fig. 2 Flowchart of the proposed DL-aided topology optimization approach

References

- [1] Yi, G., and Youn, B. D., "A comprehensive survey on topology optimization of phononic crystals," *Structural and Multidisciplinary Optimization*, Vol. 54, 2016, pp. 1315–1344.
- [2] Sigmund, O., "On the usefulness of non-gradient approaches in topology optimization," *Structural and Multidisciplinary Optimization*, Vol. 43, 2011, pp. 589–596.
- [3] Sigmund, O., and Jensen, J., "Topology optimization of phononic band gap materials and structures," *Fifth World Congress on Computational Mechanics, Vienna, Austria*, 2002, pp. 1–12.
- [4] Halkjær, S., Sigmund, O., and Jensen, J. S., "Maximizing band gaps in plate structures," *Structural and Multidisciplinary Optimization*, Vol. 32, 2006, pp. 263–275.
- [5] Halkjær, S., Sigmund, O., and Jensen, J. S., "Inverse design of phononic crystals by topology optimization," *Zeitschrift für Kristallographie-Crystalline Materials*, Vol. 220, No. 9-10, 2005, pp. 895–905.

- [6] Li, Y. F., Huang, X., and Zhou, S., "Topological design of cellular phononic band gap crystals," *Materials*, Vol. 9, No. 3, 2016, p. 186.
- [7] van den Boom, S. J., Abedi, R., van Keulen, F., and Aragón, A. M., "A level set-based interface-enriched topology optimization for the design of phononic crystals with smooth boundaries," *Computer Methods in Applied Mechanics and Engineering*, Vol. 408, 2023, p. 115888.
- [8] Hussein, M. I., Hamza, K., Hulbert, G. M., and Saitou, K., "Optimal synthesis of 2D phononic crystals for broadband frequency isolation," *Waves in Random and Complex Media*, Vol. 17, No. 4, 2007, pp. 491–510.
- [9] Bilal, O. R., and Hussein, M. I., "Ultrawide phononic band gap for combined in-plane and out-of-plane waves," *Physical Review E*, Vol. 84, No. 6, 2011, p. 065701.
- [10] Bilal, O. R., and Hussein, M. I., "Optimization of phononic crystals for the simultaneous attenuation of out-of-plane and in-plane waves," ASME International Mechanical Engineering Congress and Exposition, Vol. 54945, 2011, pp. 969–972.
- [11] Dong, H.-W., Su, X.-X., Wang, Y.-S., and Zhang, C., "Topological optimization of two-dimensional phononic crystals based on the finite element method and genetic algorithm," *Structural and Multidisciplinary Optimization*, Vol. 50, 2014, pp. 593–604.
- [12] Hussein, M. I., Hamza, K., Hulbert, G. M., Scott, R. A., and Saitou, K., "Multiobjective evolutionary optimization of periodic layered materials for desired wave dispersion characteristics," *Structural and Multidisciplinary Optimization*, Vol. 31, 2006, pp. 60–75.
- [13] Deb, K., Pratap, A., Agarwal, S., and Meyarivan, T., "A fast and elitist multiobjective genetic algorithm: NSGA-II," *IEEE transactions on evolutionary computation*, Vol. 6, No. 2, 2002, pp. 182–197.
- [14] Kudela, P., Ijjeh, A., Radzienski, M., Miniaci, M., Pugno, N., and Ostachowicz, W., "Deep learning aided topology optimization of phononic crystals," *Mechanical Systems and Signal Processing*, Vol. 200, 2023, p. 110636.