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A local radial basis function collocation method for band structure computation of phononic crystals with scatterers of arbitrary geometry

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Abstract: A numerical algorithm based on the local radial basis function collocation method (LRBFCM) is developed for the efficient computation of the derivatives of the primary field quantities. Instead of a direct calculation of the derivatives by using the partial differentiation of the shape functions as in the traditional numerical approach, the derivative calculation in the present work is performed by using a simple finite difference scheme with an introduced fictitious node. The developed algorithm is very geometrically flexible and can be easily applied to the continuity and boundary conditions of arbitrary geometries, which require an accurate derivative computation of the primary field quantities. Based on the present numerical approach, the developed LRBFCM has been applied to the phononic crystals with scatterers of an arbitrary geometry, which has not yet been reported before to the authors’ knowledge. A few examples for anti-plane elastic wave propagation are modelled to validate the developed LRBFCM. A comparison with finite element modelling shows that the present method is efficient and flexible.

Keywords: Phononic crystals, interface conditions, elastic wave propagation, band structures, eigenvalue problems, radial basis functions.

1. Introduction
Acoustic or elastic waves of a certain range of frequencies cannot propagate in periodic structures due to the periodic variation of material properties [1]. In order to evaluate the bandgaps that stop the wave propagation, different numerical methods have been applied to compute the band structures of phononic crystals, but most of the existing methods cannot efficiently undertake this challenging task. For example, a large number of elements are needed to ensure the continuity and the equilibrium conditions on solid-fluid interfaces when the conventional FEM is used [3-5]. Neglecting transverse waves in the solid parts might result in high numerical errors in the plane wave expansion method [6, 7] and the wavelet method [8, 9]. The multi-scattering theory method [10, 11] and the Dirichlet-to-Neumann map method [12, 13] are only suitable for scatterers with simple shapes such as circles and spheres. The boundary element method (BEM) [15, 16] involves singular integrals and may result in fictitious eigenfrequencies or missing of some eigenfrequencies. The generalized multipole technique [16, 17] is computationally very demanding because the band structure can only be obtained from the time domain using the Fast Fourier Transform method. The time-domain finite difference approach [18, 19] is able to consider different wave modes in solids and fluids but often has to neglect solid-fluid interactions at the interfaces. Therefore, accurate and efficient numerical methods are still needed to compute the band structures of phononic crystals.
The meshless method of the radial basis function collocation method (RBFCM) has been developed many years [23-25]. Due to the full matrix formulated in the RBFCM, the single local collocation approach is introduced, which is also known as the RBF-FD method or local RBFCM (LRBFCM) [26-30]. However, the instability caused by the Neumann boundary conditions limits its wider applications considerably [27, 31]. In order to solve this problem, special treatments were introduced to the LRBFCM for the derivation calculation. The fictitious nodes are introduced near the boundaries to increase the smooth of the solution and avoid of one side stencil [32, 33], however the fictitious nodes increase the size of the formulated matrix, and might have a limitation in the application of multi-domain eigenvalue problems; The least square method is introduced to develop LRBFCM to the phononics crystals [34, 35], but the only considered case is limited in the square lattice with square scatterers, the instability of the derivative calculation is still remain unsolved. The direct method, indirect method and fictitious node method were proposed for the derivative calculation in LRBFCM, and have been applied to phononic crystals of different problems [36-38]. However, these methods are still not easy to be applied to the phononic crystals with a complex geometry interface. By far, the LRBFCM has not yet been applied to the phononic crystals with a complex scatterer before.

In this work, a simple approach is introduced in the LRBFCM to deal with the instability caused by derivative calculation. Unlike other finite difference form introduced in LRBFCM [27, 39], the derivative calculation in this presented work is evaluated by using a simple finite difference form between the source point and one introduced fictitious node, the derivative of any direction at any node can be easily evaluated. The introduced fictitious node does not increase the size of the formulated matrix, and can greatly increase the geometric flexibility of the LRBFCM. A boundary value problem is first introduced to present the stability of this new approach. The improved LRBFCM is then applied to compute the band structures of phononic crystals with scatterers of arbitrary geometry. Two examples with anti-plane elastic wave propagation were modelled using the improved method and the results were compared by FEM models. The paper is organized as follows. The general form of LRBFCM and the new numerical technique is given in section 2. The stability tests with a boundary value problem is given in the section 3. The problem of phononic crystals are briefly introduced in section 4. The numerical results of the phononic crystals are presented and discussed in section 5, followed by some conclusions in the last section.

2. LRBFCM and the numerical technique for derivative calculation

2.1 General formulation of LRBFCM

In the LRBFCM formulation, the general solution of the field quantity \( u \) is approximated by

\[
 u(\mathbf{x}) = \sum_{m=1}^{N_s} \phi \left( \| \mathbf{x} - \mathbf{x}_m \| \right) \alpha_m ,
\]

where \( N_s \) is the total number of local nodes, \( \phi \) the RBF, and \( \alpha_m \) the unknown coefficient related to \( u(\mathbf{x}_m) \) of the local node at \( \mathbf{x}_m \), which can be calculated by
\[ \alpha_m = \varphi^{-1} \bar{u}, \]  

(2)

where \( \bar{u} = [u(x_1), \ldots, u(x_N)] \) is the vector of the field quantities of the local nodes \((m=1, N)\), \( \alpha_m = [\alpha_{1m}, \alpha_{2m}, \ldots, \alpha_{Nm}] \) is the vector of unknown coefficients, and \( \varphi = [\varphi (\|x_j - x_i\|)] \) is the RBF interpolation matrix with the size of \( N_s \times N_s \).

Considering Eq. (1), Eq. (2) can be expressed as

\[ u(x) = \sum_{n=1}^{N_s} \varphi (\|x - x_n\|) \alpha_m = \Theta \varphi^{-1} \bar{u}, \quad (3) \]

where

\[ \Theta = [\varphi (\|x - x_1\|), \ldots, \varphi (\|x - x_N\|)] \]  

(4)

In Eq. (3), \( \Theta \varphi^{-1} \) is the vector with the size of \( N_s \) that relates to local nodes. For convenience, the following definition is introduced

\[ \bar{\varphi}(x) = \Theta(x) \varphi^{-1}. \quad (5) \]

Then the field quantities given in Eq. (3) can be expressed as

\[ u(x) = \bar{\varphi}(x)^T \bar{u}. \quad (6) \]

From Eq. (6), it is easy to reformulate the vector \( \bar{\varphi}(x) \) to a global vector by inserting zeros at proper positions. For simplicity, two global vectors \( \bar{\varphi}(x) \) and \( \bar{u} \) with the size of \( N \) (the number of global nodes) are defined by mapping the local ones with the size of \( N_s \) as

\[ \text{local } \bar{\varphi}(x) \Rightarrow \text{global } \bar{\varphi}(x), \]

\[ \text{local } \bar{u} \Rightarrow \text{global } \bar{u}, \quad (7) \]

where \( \bar{u} = [u(x_1), \ldots, u(x_N)] \) is the vector of field quantities in the global domain. The global vector \( \bar{\varphi}(x) = [\varphi_1(x), \ldots, \varphi_N(x)] \) is a sparse vector related to the local vector. Using the relationships (7), Eq. (6) can be expressed as

\[ u(x) = \bar{\varphi}(x)^T \bar{u} = \bar{\varphi}(x)^T \bar{\varphi}(x)^{-1} \bar{u}, \quad (8) \]

where the unknown field quantity vector \( \bar{u} \) can be determined from governing partial differential equations and boundary conditions. \( \bar{\varphi}(x) \) is related to the partial differentiation of \( \Theta(x) \) while \( \varphi^{-1} \) is a constant matrix, i.e.,
\[
\frac{\partial u(x)}{\partial x_i} = \frac{\partial \tilde{\phi}(x)}{\partial x_i} u \Rightarrow \frac{\partial \tilde{\phi}(x)}{\partial x_i} u = \frac{\partial \Theta(x)}{\partial x_i} \phi^{-1} u,
\]

(9)

The function \( \tilde{\phi}(x) \) obeys the Kronecker-delta property, \( \tilde{\phi}_k(x_m) = \delta_{km} \) or

\[
\tilde{\phi}(x_m) = [\tilde{\phi}_1(x_m) = 0, \ldots, \tilde{\phi}_m(x_m) = 1, \ldots, \tilde{\phi}_N(x_N) = 0]
\]

and hence

\[
u(x_m) = \tilde{\phi}(x_m) u = \sum_{k=1}^{N} \phi_k(x_m) u(x_k) = \sum_{k=1}^{N} \delta_{km} u(x_k) = u(x_m),
\]

(10)

where the subscript \( m \) denotes the \( m \)th element of a vector, the corresponding field quantity at the \( m \)th node \( x = x_m \).

2.2 The numerical technique for derivative calculation

The instabilities of the LRBFCM may stop the application of the LRBFCM. Many numerical approaches, such as residual based error [40,41], least-squares method [42,43], have been applied to deal with the instability of the collocation method [44, 45]. Instabilities of the LRBFCM may relate to shape parameter, local nodes, nodes distribution and so on. One of the key instabilities caused by the LRBFCM is the derivative calculation. In the proposed numerical approach of solving derivative, a fictitious node or ghost node is used as shown in Fig. 1. This fictitious node is interpolated by using the local nodes, and thus does not increase the size of the formulated matrix. The derivative of \( \partial u / \partial n \) can be calculated in two steps. Firstly, the field quantity values on the fictitious node is interpolated using the information of the real nodes nearby, as shown in the circular area in Fig. 1. Hence we have

\[
u(\tilde{x}) = \tilde{\phi}(\tilde{x}) u_{\tilde{x}},
\]

(11)

where \( u_{\tilde{x}} = [u(x_1), \ldots, u(x_{N_f})]^T \) are the values of the field quantities at real nodes in the local domain, and \( \tilde{x} \) is the fictitious node that does not exist in the reality. Then the derivative can be
formulated using a finite difference form instead of the RBF trial function, by subtracting the field quantity of the source node \( x_k \). The derivative of the field quantity can be expressed as

\[
\frac{\partial u(x)}{\partial n} = \frac{u(x) - u(\tilde{x})}{ds},
\]

where \( ds \) is the distance between the source node and the fictitious node, as shown in Fig. 3. Considering Eqs. (10) and (11), Eq. (12) can be rewritten as

\[
\frac{\partial u(x)}{\partial n} = \frac{u(x) - u(\tilde{x})}{ds} = \frac{\phi(x) - \phi(\tilde{x})}{ds} u_{x_k}.
\]

As \( \tilde{\phi}(x) \) has the Kronecker-delta property \( \tilde{\phi}_k(x_m) = \delta_{km} \), Eq. (13) can be further modified as

\[
\frac{\tilde{\phi}(\tilde{x}) - \tilde{\phi}(x)}{ds} = \frac{[\phi_1(\tilde{x}), ..., \phi_l(\tilde{x}) - 1, ..., \phi_n(x)]}{ds},
\]

where \( k \) denotes the node \( x_k \) as shown in Fig. 1. In Eq. (14), the field quantity of the only fictitious node is interpolated using the local nodes in the small domain. Due to the Kronecker-delta property, the field quantity at the boundary node is given analytically in the derivative calculation, the accuracy and the stability of the derivative calculation is only related to the interpolation of the field quantity located at the fictitious node. As the distance \( ds \) is getting smaller, the accuracy of the derivative is greatly increasing in the LRBFCM. This approach combines the advantages of the RBF interpolation and the Kronecker-delta property together, the derivative can easily be solved no matter how complex is the interface or boundary.

3. The stability tests with a boundary value problem

In order to fully validate the proposed approach, a simple laplace case with a square domain is considered, as shown in Fig. 2. A uniform nodes distribution with \( 31 \times 31 \) is considered to compare the proposed approach with the traditional LRBFCM, as shown in Fig. 2. The Neumann boundary condition is considered on right boundary. The shape parameter is fixed with \( \zeta_s = 1 \), the number of local nodes from 5 to 13 are tested as shown in Fig. 3. 9 nearest local nodes are employed including the inner domain and boundary nodes. The exact solutions of \( u(x) = \sin(x)e^y \) is taken as the test function, numerical errors are given as follows

\[
\text{Errors} = \sum |E_x - E_n| / \sum |E_x|,
\]

where the \( E_x \) are the exact solution and \( E_n \) denote the numerical results. The multiquartic RBF is considered

\[
\phi = \sqrt{r^2 + \zeta_s},
\]

where \( \zeta_s \) is the shape parameter of the RBF and \( \zeta_s > 0 \).
As shown in Fig.3, the convergence rate of the proposed LRBFCM is much faster than traditional LRBFCM, the accuracy and stability of the proposed LRBFCM increases as the $d_s$ diseases. The numerical results when $d_s=10^{-3}$ show that small value of $d_s$ should be employed to keep a certain accuracy. Theoretically, smaller $d_s$ can always lead to better numerical results. However, singularity may influence numerical results as two nodes are getting close to each other.

In order to show the improvement of the proposed approach, and further discuss the influence of the $d_s$, the Neumann boundary conditions on all the boundaries, and only one single node information on the right above corner in Fig.4 is given. A disorder with the range of 0.01 is considered based on the same $31 \times 31$ uniform nodes to generate the random nodes distribution in Fig.4. The traditional LRBFCM may be difficult to solve this case due to difficulties in choosing
proper shape parameters and subdomain nodes.

Fig. 4 Nodes distribution of the considered domain

The influence of $ds$ with different shape parameters are presented in Fig. 5, where $ds$ is changing from $10^{-1}$ to $10^{10}$. Fig. 5 shows that the $ds$ introduced can greatly enhance the LRBFCM for Neumann boundary conditions. As $ds$ is decreasing before $10^{-2}$, the numerical results are getting better, this is because the accuracy of the of derivative is increasing as $ds$ is getting smaller. $ds$ between $10^{-2}$ and $10^{-6}$ always leads to good results, when $ds$ is less than $10^{-8}$ the numerical results are becoming worse. This is because of the singularity when the nodes are too close.

In general, the proposed numerical approach can well treat the Neumann boundary conditions for LRBFCM, $ds$ between $10^{-2}$ and $10^{-6}$ is suggested. Based on this approach, the LRBFCM is developed to the phononic crystals with an arbitrary sactterers, where normal derivative in a complex interface must be proper treated.

Fig. 5 The numerical results influence with different $ds$
3. Problem of Phononic crystals

Since this work is mainly focus on an arbitrary scatterer phononic crystals, governing equations and related boundary conditions are briefly presented. More the RBF formulation of phononic please refer to [36].

3.1 Governing equations

Consider a 2D phononic crystal composed of scatterers of an arbitrary shape embedded in a square matrix with the lattice constant $a$ as illustrated in Fig. 6, where $\Gamma_1$ to $\Gamma_4$ and $\Gamma_1$ to $\Gamma_6$ represent the boundaries of a unit-cell, and $\Gamma_0$ is the interface between the matrix and a scatterer. The governing equations of the anti-plane elastic waves in a homogeneous, isotropic and linear elastic solid are

$$\Delta u(x) = -\frac{\omega^2}{c_j^2} u(x),$$

(16)

where $\omega$ is the rotation frequency, $c_j = \sqrt{\rho_j / \mu_j}$ the elastic wave speed ($j=1$ for the scatterer domain $D_1$ and 2 for the matrix domain $D_2$), $\rho$ the mass density and $\mu$ the shear modulus.

![Fig. 6 Phononic crystal structures: (a1), (a2) and (a3) represent the square lattice, the square unit-cell and the first Brillouin zone; (b1), (b2) and (b3) the triangular lattice, the hexagonal unit-cell and the first Brillouin zone.](image)

3.2 Interface conditions

The continuity conditions on the interface $\Gamma_0$ are expressed as
where \( n = (n_x, n_y)^T \) is the outward unit normal vector of the scatterer.

### 3.3 Periodic boundary conditions

The periodic boundary conditions are given as

\[
\begin{align*}
\mu_1 \frac{\partial u_1(x)}{\partial n} &= \mu_2 \frac{\partial u_2(x)}{\partial n}, & x \in \Gamma_0, \\
0 \in \Gamma_x &,
\end{align*}
\]

where \( \mu = \mu_1, \mu_2 \) are the medium permeabilities, \( u_1, u_2 \) are the scattered fields in the left and right medium, respectively, \( x \in \Gamma_0 \) is the boundary surface and \( n \) is the outward unit normal vector of the scatterer.

The periodic boundary conditions are given as

\[
\begin{align*}
0 \in \Gamma_x &,
\end{align*}
\]

where \( k = (k_x, k_y)^T \) is the Bloch wave vector, \( i = \sqrt{-1} \), \( t(x) = \frac{\partial u(x)}{\partial n} \), and \( a = l_1 a_1 + l_2 a_2 \) with \((l_1, l_2) \in \mathbb{Z}^2\), where \( a_1 \) and \( a_2 \) are fundamental translation vectors of the lattices.

For the square lattice we have

\[
\begin{align*}
u(x_1 + a) &= e^{ik_x a} u(x_1), & u(x_1 + a) &= e^{ik_y a} u(x_1), \\
t(x_1 + a) &= e^{ik_x a} t(x_1), & t(x_1 + a) &= e^{ik_y a} t(x_1),
\end{align*}
\]

where \( x_1 \) \((i=1~4)\) are the nodes on the boundaries \( \Gamma_x \).

For the triangular lattice we have:

\[
\begin{align*}
u(x_1) &= u(x_1) e^{-i \frac{\sqrt{3}}{2} a}, & u(x_1) &= u(x_1) e^{i \frac{\sqrt{3}}{2} a}, \\
t(x_1) &= t(x_1) e^{i \frac{\sqrt{3}}{2} a}, & t(x_1) &= t(x_1) e^{-i \frac{\sqrt{3}}{2} a},
\end{align*}
\]

The generalized eigenvalue equation is

\[
\mu_1 \frac{\partial u_1(x)}{\partial n} = \mu_2 \frac{\partial u_2(x)}{\partial n},
\]

where \( u_1, u_2 \) are the scattered fields in the left and right medium, respectively, \( x \in \Gamma_0 \) is the boundary surface and \( n \) is the outward unit normal vector of the scatterer.

### 4 Numerical results and discussions

The present LRBFCM is validated by comparison of numerical results with those obtained from finite element modelling using COMSOL Multiphysics 5.0. There is little time difference due to different eigenvalue solvers of the LRBFCM and FEM. The generalized eigenvalue equation is
solved numerically by using the eigensolver in MATLAB. 9 local nodes are employed for both boundary and inner domain, $ds=10^{-6}$ is employed, the shape parameter is choosen as 1. Scatterers made of gold (Au) and aluminium (Al) embedded in an epoxy matrix are modelled, respectively. The material constants are $\rho_1=19500\text{kg/m}^3$ and $c_1=1239\text{m/s}$ for Au and $\rho_1=2730\text{kg/m}^3$ and $c_1=3145\text{m/s}$ for Al, respectively. $\rho_2=1180\text{kg/m}^3$ and $c_2=1161\text{m/s}$ for the epoxy. This leads to acoustic impedance ratio $Z=\rho_1 c_1/\rho_2 c_2=17.64$ for Au and $Z=6.46$ for Al, respectively.

4.1 Numerical results

Square lattice

The square lattice with a scatterer of star shape and its first Brillouin zone with 225 points are shown on the left and right hand side of Fig. 7 respectively. The band structures are obtained by sweeping all the first Brillouin zone points.

![Square lattice and first Brillouin zone](image)

Fig. 7 Square lattice (left) and its related first Brillouin zone (right)

An FE mesh with 2737 degrees of freedom and 1348 elements are used for comparison with the LRBFCM with 2585 degrees of freedom and 2454 nodes, as shown in Fig. 8 and Fig. 9, respectively. The corresponding band structures of the Au scatterer embedded in the epoxy matrix are shown in Fig. 10 and Fig. 11, respectively. It is clear that the present results agree quite well with the FEM results. The band gap can be easily calculated from the first and second band of eigenvalues. Fig. 12 and Fig. 13 show the band structures of the Al scatterer embedded in the epoxy matrix using the FEM and the LRBFCM, respectively. Again an excellent agreement can be seen, and different material properties do not affect the accuracy of numerical results.
Triangular lattice

The triangular lattice with a star shape scatterer is shown in Fig. 14 with 165 points used in the first Brillouin zone. For this example, 1487 degrees of freedom with 408 elements are employed in the FE mesh, and 2181 degrees of freedom with 2055 nodes used in the LRBFCM, as shown in
Fig. 15 and Fig. 16, respectively. Fig. 17 and Fig. 18 show the band structures of the Au scatterer case from the FEM and LRBFCM, respectively. The results for the Al scatterer case are shown in Fig. 19 and Fig. 20, respectively. All the results are in excellent agreement.

Fig. 14 Triangular lattice (left) and its first Brillouin zone (right)

Fig. 15 FEM mesh
Fig. 16 Nodes distribution in RBF

Fig. 17 Band structures of Au/Ep using FEM
Fig. 18 Band structures of Au/Ep using LRBFCM
4.3 Comparison and analysis

The CPU times and errors of the FEM and the LRBFCM for the above numerical examples are given in Table 1. The lowest ten eigenvalues are compared and the errors are defined as

\[ \text{Errors} = \sum |E_f - E_r| / \sum |E_r|, \tag{25} \]

where \( E_f \) is the FEM result using COMSOL\textsuperscript{TM} Multiphysics and \( E_r \) the result of LRBFCM implemented in a Matlab code. All the simulations are run on a laptop with Intel(R) Core(TM) i7-4510U, 2.00 GHz CPU and 8 GB RAM.

Table 1 shows that the performance of the LRBFCM is much better than that of the FEM in general. Although more degrees of freedom are purposely employed in the LRBFCM for the examples, the computing time is much less than that required by the FEM, with more than 90% savings in all the cases considered here. The high efficiency of the present LRBFCM is attributed to the fact that it is based on a strong-form formulation of partial differential equations and does not need any numerical integration for computing the system matrices. The errors in Table 1 also shows that the improved LRBFCM can deal with the arbitrary interface very well.

5. Conclusions

In this paper, an improved numerical approach based on the LRBFCM has been developed to accurately compute the normal derivatives of field quantities, and thus the continuity conditions of arbitrary geometry interfaces can be treated more properly, the LRBFCM can be developed to the phononic crystal with scatterers of arbitrary geometry. Numerical results show that the improved LRBFCM is capable of very efficiently computing the band structure of phononic crystals with scatterers of arbitrary geometry. Due to its advantages in dealing with complicated boundary or interface shapes, the improved LRBFCM can be extended to simulate other problems such as acoustics, solid-fluid interaction, crack propagation and hydrodynamics with moving boundaries.
Table 1 Comparisons of computing time and accuracy for the phononic crystals

<table>
<thead>
<tr>
<th>Lattice form</th>
<th>Square</th>
<th>Triangular</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Material properties</strong></td>
<td><strong>Au/Ep</strong></td>
<td><strong>Al/Ep</strong></td>
</tr>
<tr>
<td><strong>RBF</strong></td>
<td>Degrees of freedom</td>
<td>2585</td>
</tr>
<tr>
<td></td>
<td>Time spent [s]</td>
<td>88.8</td>
</tr>
<tr>
<td><strong>FEM</strong></td>
<td>Degrees of freedom</td>
<td>2055</td>
</tr>
<tr>
<td></td>
<td>Time spent [s]</td>
<td>1003</td>
</tr>
<tr>
<td><strong>Comparison</strong></td>
<td>Errors</td>
<td>0.00698</td>
</tr>
<tr>
<td></td>
<td>Time saving</td>
<td>91.14%</td>
</tr>
</tbody>
</table>

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