Photonics Bandgap Computations using Novel Periodic Meshless Methods

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Abstract ─ Although many numerical methods have been developed to calculate photonic bandgap structure properties, but always improvement in numerical methods is necessary to have more efficient, accurate and flexible techniques. In the present work, novel periodic meshless shape functions including so-called direct and radial shape functions are presented. The meshless approaches, based on these periodic shape functions as real-space methods, can be used for simulation of periodic structures, like photonics bandgap structures, straightforwardly. The results on band structures derived from the proposed methods are then presented, discussed and compared with those available in the literature, and a very good agreement is seen. It shows that the proposed techniques are very promising to be robust techniques in the simulation of periodic structures such as photonic problems.

Index Terms ─ Meshless methods, photonics bandgap, periodic shape functions.

I. INTRODUCTION

Accurate simulation of bandgap structures is indispensable development of various opto-electromagnetic devices [1], [2]. The major groups of the band structure materials have periodic constructions. It is common to analyze periodic geometries by assuming that the structure extends to infinity in one or more directions. Sometimes, this is done in order to simplify the analysis. But the infinite structure can also be viewed as the ideal structure because there are no truncation edges present to possibly degrade the electromagnetic performance. When the structure extends to infinity, it is possible to analyze the electromagnetic performance by considering only one period of the geometrical pattern, i.e. a unit cell. Periodicity and antiperiodicity geometry aspects can be able to reduce the complexities of studied domain of the device [3].

One of the well-known techniques in analyzing photonics bandgap problems is the plane wave method. But this conventional technique has convergence problem arising from the abrupt change in the value of dielectric function across

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the interface between matrix and inclusion [4]. Thus, real-space numerical methods have also been tried for more efficient calculations of photonic band structures. Among them, the periodic finite-difference time-domain (FDTD) method [3] and the periodic finite element method (FEM) [5] are commonly used. The main advantage of using the FEM for infinite periodic analysis compared to the FDTD is the ease of use unstructured grids that can model complex structures with large variation in length scale as well as elements that can better conform to curved boundaries. The computation accuracy of the FEM, however, depends upon the quality of the used mesh. In addition, the meshing process is also known as a very complex and time consuming task.

Unlike the conventional element-based numerical methods, meshless methods expand the field quantities around a set of scattered nodes that can be randomly placed spatially in a problem domain [6]. As a result, their numerical accuracies are independent on the connectivity laws of the grid nodes. In addition, any irregular shape of interface between materials is easily recognized in meshless modeling by simply putting nodes along the interface, e.g., photonic crystals or other metamaterials which they can have any arbitrary shape dielectrics. One of the other unique potential applications for meshless methods is that the methods may be well-suited to adaptive computation which is needed in some devices like liquid crystal materials. Owing to these distinctive features, meshless methods have been introduced as robust and flexible computational methods in a variety of engineering areas, confidently.

To our best knowledge, a few studies have been done on using meshless methods for analyzing periodic structures. This is due to this fact that the shape functions are usually global in the conventional meshless methods and introducing periodic boundary conditions are inherently different from other methods. So, for solving this problem in meshless approach, by implementing periodic shape functions, periodic boundary conditions can be imposed spontaneous. In [7], the author proposed a technique for constructing periodic mean least-square (MLS) shape functions. But as it is known, MLS shape functions do not have the delta function property and thus imposing essential boundary conditions would not be performed, straightforwardly. On the other hand, recently, some other approximations or shape functions, called direct shape functions (DSFs), have been proposed which can be created directly and be more efficient [8], [9]. In this work, a new technique is introduced to generate periodic meshless shape functions. The proposed technique is applied to DSFs and shape functions used in radial point interpolation method (RPIM) [6] to obtain periodic shape functions. Then, the proposed periodic shape functions are employed to calculate the eigenvalues and the eigenfunctions of the electric field in a photonic bandgap structure.

II. PERIODIC SHAPE FUNCTION CONSTRUCTION

Here, we introduce a simple technique to construct inherently suitable shape functions for periodicity. Our proposed technique is enforced on the weighting or basis functions then it would be affected on the shape functions, straightforwardly. In Fig. 1, a periodic domain with generic parallelogram cell is shown. The lattice vector $\vec{L}$ is denoted by

$$\vec{L} = n_1\vec{a}_1 + n_2\vec{a}_2 \tag{1}$$

where $\vec{a}_1$, $\vec{a}_2$ are primitive lattice vectors and n_1, n_2 are integers. In meshless approach, a unit cell is discretized by a set of nodes $i = 1,2,\cdots,N$. Because of periodic nature of the structure, the field will change in a periodic manner in the problem domain. So

$$u(X) = u(X + \vec{L}) \tag{2}$$

for any point X in the unit cell. In periodic approach, dual points of a node such as X should be found, first. It can be easily performed using the components of the lattice vector as

$$X'_{pq} = X + pn_1\vec{a}_1 + qn_2\vec{a}_2 \tag{3}$$

where $p,q = -M,-M+1,\cdots,M-1,M$ and M is a large integer. X'_{00} is actual point and the others X'_{pq} are named dual points. So in fact, there are too many dual points for each point in the unit cell. But, it should be noted that only those dual points which are located in the neighbour cells are usually important. For example, in a tetrahedron cell, there are eight neighbour cells. In the

parallelogram cell, the lattice vector has two components $\vec{a}_1$ and $\vec{a}_2$ and each point has eight

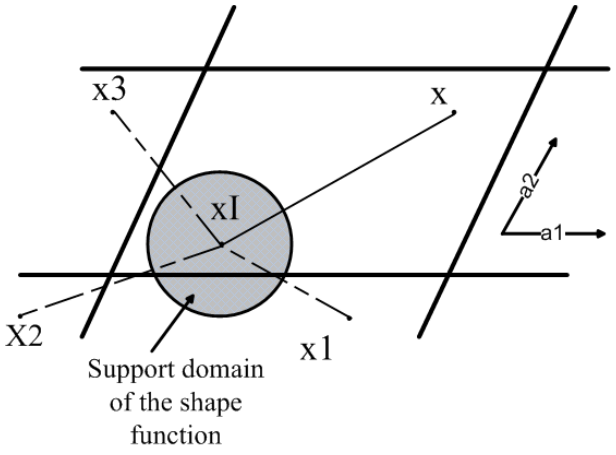


Fig. 1. A generic point in one of the shape function support domains in a unit cell. An actual point X and its three dual points, i.e. X_1, X_2, X_3, are shown. To determine the periodic shape function corresponding to X_I in point X, the shortest distance or the shortest line, i.e. dash line shown in the figure, must be used.

dual points, i.e., 3^2-1 in the neighbour cells. These points can be obtained from (3) by setting $p,q=-1,0,1$. It should be carefully noted, although, in a generic periodic structure like Fig. 1, there are some dual points, but generally only a few numbers of them must be considered. In fact, the others have a considerably remote distance from X_I which is obvious and recognizable. For example in Fig. 1, for point X there are eight dual points in the neighbour cells, but only three nearer dual points should be considered. For example, let the considered point be in the lower left corner of the tetrahedron. It is clear that the dual point which is in the top cell, does not have a distance smaller than the actual distance.

According to the lattice structure, the number of dual points is clear and we cannot increase or decrease them. Also, the number of dual points considered must be obtained carefully and exactly.

As it is known, in the meshless methods corresponding to each scattered node, there is a weighting or basis function $W_i(X)$. For example, in direct meshless method proposed in [8] it is as

$$W_i(X)=\exp(-\alpha|X-X_i|) \tag{4}$$

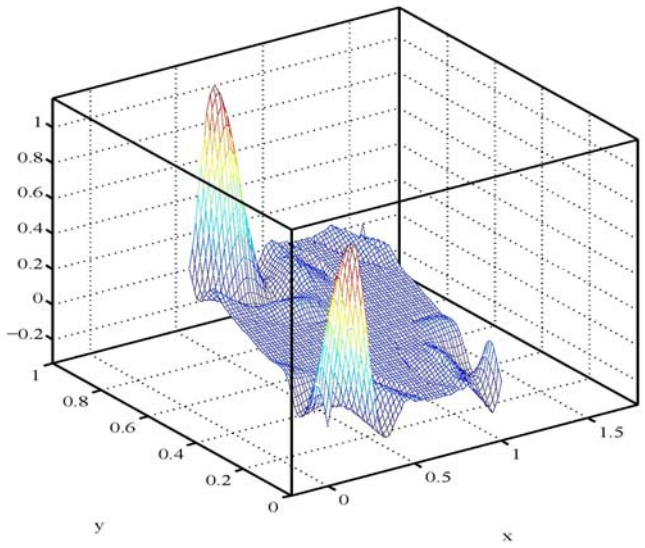
where X is the vector of space coordinates, i.e. $X^T=[x,y]$ (for 2D problems), and X_i is the space coordinate of the node that related to the weighting function. α is a positive independent coefficient. In proposed approach to have a periodic weighting function, a modification on (4) should be performed. By introducing

$$X_{nearest}=X_{nm} \quad \text{if} \quad |X_{\text{mn}}-X_i|\le|X_{\text{pq}}-X_i| \tag{5}$$

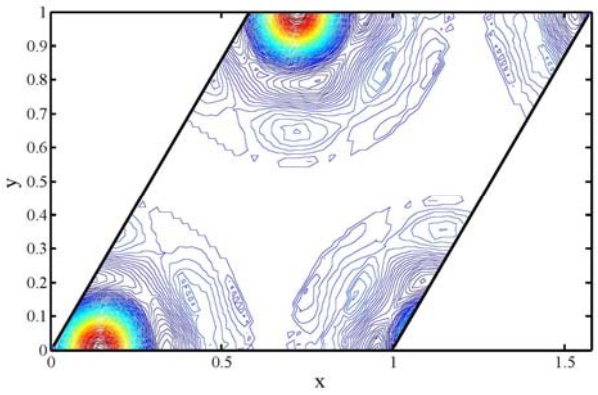
Then a periodic weighting function can be proposed as

$$W_i(X)=\exp(-\alpha|X_{nearest}-X_i|) \tag{6}$$

Above formula means that to construct a periodic shape function at a generic point X, first, the points of X should be obtained and then the nearest point to the center of the shape function, according to (5), would be used instead of X in the conventional basis function formula. This idea comes from this fact that the field in nonperiodic structures at X_i has a small influence on aloof points from X_i; or in other words, the shape functions $N_i(X)$ would be vanished far away from X_i. Whereas in periodic structures, an aloof point may have a dual point which can be closed to X_i. On the other hand, because any point has the same value of its dual points, so its dual distance can be replaced instead of the actual distance in formulas.



(a)



(b)

Fig. 2. The shape function corresponding to a node near the lower left corner. a) 3D demonstration. b) Equal-value contour plot.

This approach can be applied to other meshless shape functions, straightforwardly. In the case of periodic local radial point interpolation method (RPIM) shape functions [6], the support domain of the point of interest must be first determined. For example for a node in the near lower left corner of a lattice, we first find scattered nodes in the support domain of node *X*, then node *X* is translated to $X+\vec{a}_1$ and node search is applied again. The same procedure is repeated for $X+\vec{a}_2$ and for $X+\vec{a}_1+\vec{a}_2$ where $\vec{a}_1, \vec{a}_2$ are primitive lattice vectors. After determining the support domain, the periodic RPIM approximation can be written as

$$u(X) = \sum_i a_i R_i(X) \qquad (7)$$

where $R_i(X)$ is the regular radial basis function except for the definition of distance where the new definition of distance discussed above is used, and a_i are unknown coefficients. By letting *u(X)* passes through each scattered node in the support domain, the unknown coefficients can be determined.

Here, the introduced technique is used to make periodic local radial shape function. Figure 2 shows one of the shape functions near the lower left corner of the parallelogram. Periodic nature of the shape function is appeared, clearly, in this figure. The shape function has non-vanishing values near all the four corners as a result of dual point technique. By using these periodic shape functions, meshless method can simulate an indicator unit cell without any other boundary conditions on the periodic boundaries.

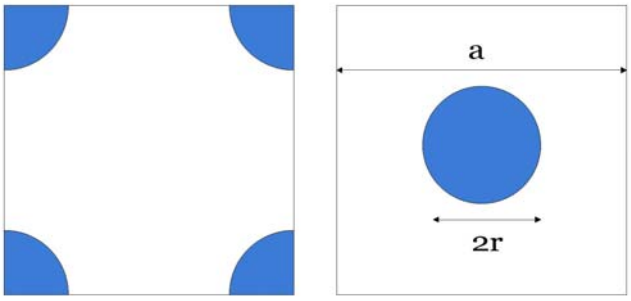


Fig. 3. Two different configurations for the unit cell used to model the desired structure.

III. NUMERICAL EXAMPLE

In this section, we attempt to validate our proposed techniques through numerical experiment by simulating a well-known problem in periodic structures literature. The problem considered is an array of dielectric rods in free space periodically arranged [1]. The structure is assumed to be infinite in *x* and *y* directions both, and is infinitely long in *z* direction. Since the dielectric rods are periodically arranged, and because the structure is infinite in both *x* and *y* directions, we can simply model it by a unit cell to which the proposed periodic meshless methods are employed to calculate its frequency band structures. This problem can be considered as a good test to measure the technique capability in simulating periodic and inhomogeneous regions.

According to the Floquet-Bloch theorem, each components of the electromagnetic fields can be expressed by the product of a periodic function *u(X)*, where *X* is spatial coordinate, and a plane wave with the wave vector $\vec{k}$, such as [7]

$$\varphi(X) = u(X)e^{-i\vec{k}.X} \qquad (8)$$

By considering the periodic nature of the wave propagation, problem of obtaining electromagnetic fields is reduced to solving two equations for *u(X)*. For TE mode

$$-\left(\nabla + i\vec{k}\right).\frac{1}{\varepsilon(X)}.\left(\nabla - i\vec{k}\right)u(X) = \lambda u(X) \qquad (9)$$

and for TM mode

$$-\left(\nabla + i\vec{k}\right)\left(\nabla - i\vec{k}\right)u(X) = \varepsilon(X).\lambda u(X) \qquad (10)$$

where $\lambda = (\omega/c)^2$, c is the light velocity and ε is the relative permittivity of the medium.

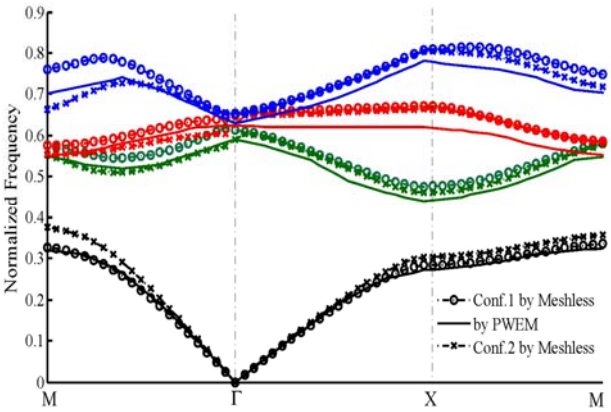


Fig. 4. Meshless results on band structures of square lattice composed of circular rods calculated by the periodic DSF for two configurations (TM mode).

In the meshless method, the field function, i.e., $\varphi(X)$ or *u(X)*, would be approximated

$$\widetilde{u}(X) = \sum_{i=1}^{N_p} a_i . \psi_i(X) \tag{11}$$

where a_i are unknown constants, N_p denotes the number of nodes and ψ_i are periodic shape functions. Manipulations after putting equation (11) into equations (9) and (10) and forming Galerkin's formulations for them, result in matrix eigenequations as

$$[A][a] = \lambda [B][a] \tag{12}$$

where for TE mode

$$A_{ij} = \int_\Omega \frac{1}{\varepsilon(X)} \left(\nabla + i\vec{k}\right)\psi_i(X).\left(\nabla - i\vec{k}\right)\psi_j(X) d\Omega$$
$$B_{ij} = \int_\Omega \psi_i(X).\psi_i(X) d\Omega \tag{13}$$

and for TM mode

$$A_{ij} = \int_\Omega \left(\nabla + i\vec{k}\right)\psi_i(X).\left(\nabla - i\vec{k}\right)\psi_j(X) d\Omega$$
$$B_{ij} = \int_\Omega \varepsilon(X)\psi_i(X).\psi_i(X) d\Omega \tag{14}$$

The radius of the circular cross section, as shown in Fig. 3, is $r = 0.2a$ for this example. Dielectric constants are $\varepsilon_m = 1.0$ and $\varepsilon_1 = 8.9$ for matrix and rods, respectively. According to Bloch's state in periodic structures, the wave numbers in the Brillouin zone are only needed to be considered.

We use two different unit cells for this problem, one configuration with a rod in the center of the cell (Conf. 1) and in the other one the unit

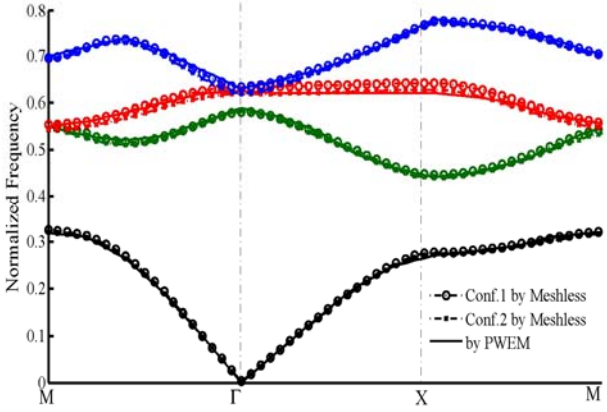


Fig. 5. Meshless results on band structures of square lattice composed of circular rods calculated by the periodic RPIM for two configurations (TM mode).

cell is chosen so that one quarter of four rods are in each corner of the lattice (Conf. 2), as shown in Fig. 3. Since these two problems are similar to each other, we expect that the frequency band diagrams obtained by applying periodic meshless methods to these two unit cells be the same, too. The results will show it is indeed the case. It can be considered as an initial criterion of the accuracy of the results. In this study we have used multi-quadrics (MQ) RPIM shape functions with shape parameters chosen as *q=0.98* and $\alpha_c = 0.5$ [6]. Moreover, the problem domain is discretized by *417* nonuniform meshless nodes. For DSF approach, the shape parameter $\alpha = 3/d_c$, where d_c is the average nodal spacing, is chosen with the same meshless nodes [8].

In this case, there exists a wide bandgap in TM modes as known in literature [7]. Meshless results on band structures also confirm the wide bandgap in TM modes as shown in Figs. 4 and 5 for both DSF and RPIM approaches, respectively. In these diagrams, the normalized frequency is drawn for different modes versus wave number, i.e., $\vec{k}$, in Brillouin zone. The results have a good agreement with those obtained by other methods such as the plan wave expansion method (PWEM) [10]. Although, the DSF meshless method accuracy is less than the accuracy of the RPIM meshless method, its simulation time is better than RPIM

method as known as one of the advantages of direct meshless methods [8], [9]. Table 1 illustrates the consuming time for shape function construction in two comparable methods, the proposed method and the RPIM approach.

Table 1: Consuming time for two different meshless approach

	Computational time (sec)	
Number of nodes	**RPIM method**	**Direct method**
289	5	2
361	10	3
441	25	7
529	58	13
625	110	20

It can be seen, when the number of nodes increases, the RPIM method processing time increases, extremely. All simulations were performed on the same PC with a CPU of 2.4 GHz and a RAM of 2 GB.

IV. CONCLUSION

We have presented successfully a new 2D meshless method applicable to analyze any infinite periodic structures, like photonic crystals. The periodic radial and direct shape functions, as two advanced meshless shape functions, based on the proposed approach were introduced and a 2D photonic crystal structure was simulated. In this approach, any complex dielectric boundaries can be modeled only by putting nodes on the boundaries, effortlessly. The photonic bandgap structure was analyzed and the obtained results matched well with the reference solutions. It thus demonstrates that the periodic meshfree shape functions implemented are very efficient for the problems of periodicity. The periodic approach has been presented in 2D quadrilateral cell, but generally 3D cells could be possible.

Nevertheless, this paper presented a simple bandgap problem. But more complicate problems can be investigated in the future such as photonic crystals with nonlinear and anisotropic materials or application of the time-domain meshless method in photonic structures, etc. In the other words, the proposed method is applicable to each periodic structure with no limitations.

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