Comparison of Nonorthogonal FDTD and Yee's Algorithm in Modelling Photonic Bandgap Structures

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Abstract

Finite-Difference Time-Domain (FDTD) method has been widely used to study Photonic Bandgap (PBG) structures. However, staircasing approximation employed by Yee's scheme for curved structures is noted to cause numerical errors when the wavelengths of interest are relative small with regard to the grid size. Consequently a high spatial resolution is required in the conventional Yee's FDTD scheme. Nonorthogonal FDTD (NFDTD) method uses a conformal grid to discretize curved structures and hence requires less computer memory in the simulation. The trade-off is the late time instability inherent in the NFDTD method. In this paper, the Yee's algorithm and NFDTD are compared in modelling the photonic bandgap structures in terms of mesh sizes, numerical accuracy and the requirements on spatial resolution.

1. INTRODUCTION

Photonic Bandgap (PBG) structures which are also termed as Photonic Crystals or Electromagnetic Bandgap (EBG) structures are periodically structured artificial electromagnetic media. They generally possess band gaps, a range of frequency in which EM waves cannot propagate through the structure. PBG studies have attracted wide attention in both physics and engineering societies [1,2].

So far, PBG structures have been extensively studied using various numerical methods including the Plane Wave Expansion (PWE) method [3,4,5], the Finite-Difference Time-Domain (FDTD) method [6], the Korringa-Kohn-Rostoker (KKR) or multiple scattering approach [7], the Transfer Matrix Method (TMM) [8,9] and the generalized Rayleigh Identity Method [10] *etc*. Among them, the FDTD method is most popular because of its simplicity in algorithm and capability to model complex structures with wide frequency band solutions. In previous FDTD approaches, an overwhelming majority is based on the Yee's scheme [11-13], using uniform orthogonal meshes. There is also an alternative FDTD approach developed in the nonorthogonal coordinate system [15], in which the dispersion diagram is obtained using a uniform rhombic grid in order to model a rhombic unit cell. In that approach, the formulas are derived from the conventional Yee's scheme with adjustments for the fixed skewed angle in the grid. However, when the curved unit cell element is considered, staircasing approximation is employed, either with an orthogonal grid [11-14] or with a rhombic grid [15]. It is anticipated that the staircasing approximation will cause numerical errors when the wavelength of interest is small with regard to the grid size. Consequently, a dense grid with high spatial resolution is required and hence leads to extensive computation with large computer memory requirement.

On the other hand, the nonorthogonal FDTD (NFDTD) scheme originated by Holland in 1983 [16] uses structured meshes when modelling curved structures. Compared to the staircase FDTD scheme, fewer meshes are needed to represent the curved or oblique boundary of electromagnetic structures. However, it has been reported that the NFDTD scheme suffers the late time instability which is inherent in the algorithm [17].

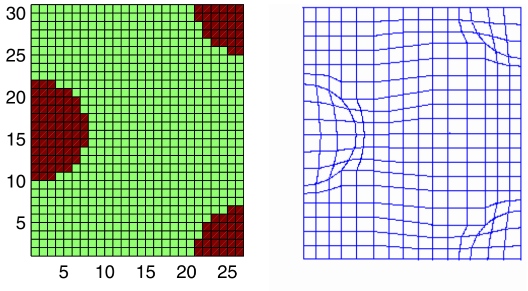
In this paper, an infinite structure of metallic cylinder rods loaded periodically in free space is modelled in terms of unit cells using both the Yee's FDTD and NFDTD algorithms. Dispersion diagrams of the PBG structure are plotted and compared using the two aforementioned algorithms in terms of numerical accuracy on frequency results and its requirements on the spatial resolution.

2. NUMERICAL SIMULATION

A. Model Parameter

Two types of unit cell namely square and triangular/rhombic lattice are considered in this paper in both TE and TM polarization respectively. The unit cell element is a metallic rod with the ratio of the radius (r) to the lattice constant (a) (r/a) 0.2. Fig.1 shows an example of triangular lattice meshed using 30×26 cells in the Yee's FDTD grid and 18×15 cells in the NFDTD grid.

The structures are fed with a modulated Gaussian pulse at a random feeding point with different normalized central frequencies in various numerical experiments. The EM fields at random points are monitored and the temporal results are processed by Fourier Transformation. Dispersion diagrams of the modelled PBG structures are validated using results in [18]. Dispersion diagrams from the Yee's and NFDTD algorithms with different mesh sizes (spatial resolution) are compared to evaluate the performance of the two algorithms.



(a) (b)

Fig. 1 Mesh Schemes for a triangular/rhombic unit cell of the metallic PBG structures. (a) in FDTD grid; (b) in NFDTD grid;

B. Comparison of the Dispersion Diagrams

In Fig.2, the dispersion diagrams of the TE modes for the triangular/rhombic lattice feeding at normalized frequency equals to 1 from the Yee's and the NFDTD algorithms are shown as an example. It is observed that for this frequency band (normalized central frequency equals to 1), the Yee's FDTD results are convergent when a grid with 30 cells or more per wavelength is used. It is noticed that a grid with 18 cells per wavelength can not result in the same diagram due to the inadequate spatial resolution. However, using the NFDTD algorithm, a grid of 18 cells per wavelength can give the same accuracy as that from the staircasing FDTD with higher spatial resolutions.

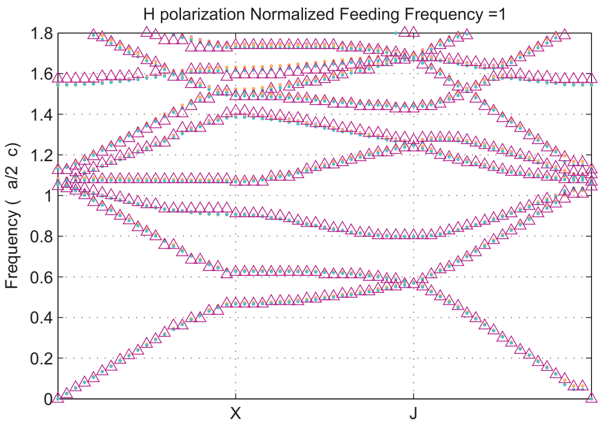


Fig. 2 The comparison of the dispersion diagrams from Yee's and NFDTD algorithms. Dots: Yee's FDTD; Triangles: NFDTD.

The same PBG structure is excited with a higher normalized frequency which equals to 2 to investigate the high frequency performance of the two algorithms. For this frequency, a spatial resolution of 15 cells per wavelength is not enough for the Yee's algorithm while the NFDTD with a resolution of 9 cells per wavelength demonstrate a maximum error of 1.4% below normalized frequency 1.5 and an error of 2.4% in the frequency band of 1.5-2.5. As is the same in the conventional Yee's FDTD algorithm, a denser NFDTD grid can offer even better accuracy than a coarse one. The dispersion diagrams of the TE modes for the triangular/rhombic lattice from Yee's algorithm (40 cells per wavelength, mesh size: 80×69) and NFDTD algorithm (15 cells per wavelength, mesh size: 30×26) are plotted and compared in Fig. 3. They show good agreement up to normalized frequency 3.

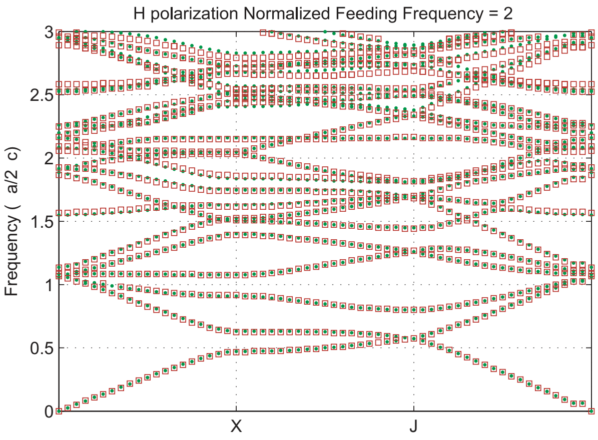


Fig. 3 The dispersion diagrams of the triangular/rhombic lattice (TE modes) from the Yee's and NFDTD algorithm with normalized feeding frequency of 2. Dots: Yee's FDTD, mesh size 80×69, 40 cells per wavelength; Square: , mesh size 30×26, 15 cells per wavelength.

Further numerical experiments with higher feeding frequency also show that using the conventional Yee's FDTD algorithm, a denser grid is required compared with the NFDTD algorithm to get the same level of accuracy in any frequency band.

C. Requirement on Spatial Resolution

Figure 4 is to compare the NFDTD results for different spatial resolution for a high feeding frequency. In this way the error rate on a coarse mesh is investigated. The normalized feeding frequency is chosen as 3, which means

$$\frac{w_f \cdot a}{2 \cdot \pi \cdot c} = \frac{a}{\lambda_{ff}} = 3$$

in which w_f is the feeding frequency, a is the lattice constant, c is the speed of light in free space, and λ_{ff} is the wavelength of the feeding frequency in free space. So for this frequency, the grid size is $\frac{\lambda_{ff}}{6}$ for mesh size 18×15 (6 cells per wavelength) and $\frac{\lambda_{ff}}{16}$ for mesh size 48×42 (16 cells per wavelength). More details with other spatial resolutions can be checked in table 1.

The diagram from mesh size 48×42 (16 NFDTD cells per wavelength for the central frequency) is taken as a reference because of its higher spatial resolution. The difference of the two results is under 0.92% from normalized frequency band 0 to 1.5; under 2.13% from normalized frequency 1.5 to 2 and under 5.5% for normalized frequency 2 to 3.

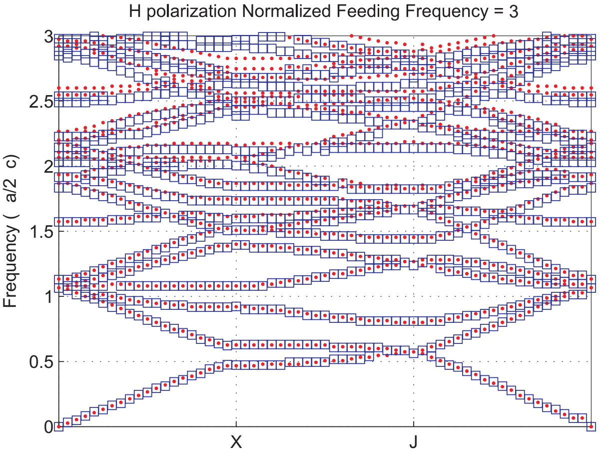


Fig. 4 Comparison of dispersion diagrams for different NFDTD spatial resolution for normalized feeding frequency of 3. Dots: mesh size 48×42 (16 cells per wavelength); Square: mesh size 18×15 (6 cells per wavelength).

TABLE 1: CAPABILITY OF THE YEE'S FDTD AND NFDTD ALGORITHMS UNDER DIFFERENT SPATIAL RESOLUTIONS

Mesh Size	Normalized frequency (a/λ_{ff})		
	1	2	3
26×23 (Yee's FDTD) / 18×15 (NFDTD)	NFDTD ($\frac{\lambda_{ff}}{18}$)	NFDTD ($\frac{\lambda_{ff}}{9}$)	NFDTD ($\frac{\lambda_{ff}}{6}$)
30×26	Yee's /NFDTD ($\frac{\lambda_{ff}}{30}$)	NFDTD ($\frac{\lambda_{ff}}{15}$)	NFDTD ($\frac{\lambda_{ff}}{10}$)
50× 43 (Yee's FDTD) / 48×42 (NFDTD)	Yee's ($\frac{\lambda_{ff}}{50}$) / NFDTD ($\frac{\lambda_{ff}}{48}$)	Yee's ($\frac{\lambda_{ff}}{25}$) / NFDTD ($\frac{\lambda_{ff}}{24}$)	NFDTD ($\frac{\lambda_{ff}}{16}$)

Table 1 shows the capability of the two algorithms under different spatial resolutions to get results with minor (less than 6%) errors. The contents of the table show the capable algorithm(s) followed by the grid size in brackets. It shows that the NFDTD grid can be 4 times bigger as that of the Yee's scheme to achieve a similar performance.

D. Lower Unexpected Modes from a Coarse Yee's Grid

Figure 5 shows what happens when the spatial resolution is not enough in both Yee's FDTD algorithm and NFDTD algorithm. Frequency spectra of Γ are calculated using Yee's FDTD with meshes of 15 cells per wavelength (size 30×26) and NFDTD with meshes of 6 cells per wavelength (size 18×15) respectively and are compared with the Yee's FDTD with meshes 40 cells per wavelength (size 80×69). Both the low spatial resolution results show errors on higher frequency band (higher than 1.8). However, in the Yee's FDTD spectra, there are unexpected modes in lower frequency band (lower than 0.5) for this model. This is not seen in NFDTD results with an even lower spatial resolution.

The unexpected lower modes observed in the Yee's coarse grid model for the metallic cylindrical rod can be explained as such: some modes are degenerated and others are spurious modes, all of which are caused by numerical inaccuracy when the circle structure is meshed using a staircasing grid.

This comparison, again, verifies that NFDTD algorithm can provide more reliable results at lower frequency band with a very low spatial resolution because of its capability of model curved structure more accurately in a conformal way. This is beneficial not only in terms of computer memory requirement, but also in providing a more robust algorithm which delivers accurate results when knowledge of the maximum frequency involved is inadequate and when modelling some complex problems.

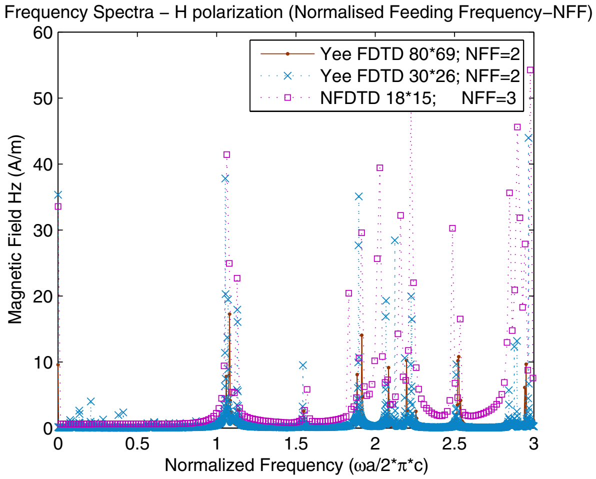


Fig. 5 Frequency Spectra for the same k vector from the Yee's FDTD and NFDTD algorithms under low spatial resolution.

3. CONCLUSION

In this paper, dispersion diagrams of a two-dimensional PBG structure of metallic cylinder rods periodically loaded in free space are obtained using both the conventional Yee's and the NFDTD algorithms. The triangular/rhombic lattice and TE polarisation is chosen for demonstrating the comparison. Similar results are observed for TM polarisation and for square lattice which are not shown here. The comparison of the frequency results shows that Yee's FDTD algorithm requires a higher spatial resolution (minimum 25 cells per wavelength) to reduce the inaccuracy in modelling and the numerical dispersion caused by staircasing approximation, while NFDTD is able to model the curved structure more accurately with a much lower spatial resolution (minimum 6 cells per wavelength). For this set of experiments, the NFDTD grid can be 4 times bigger as that of the Yee's scheme to achieve similar numerical accuracy. Consequently, the requirement on the computer memory is alleviated when using the NFDTD scheme. At the same time, when the spatial resolutions are low in both algorithms, a coarse NFDTD grid can provide reasonable accurate results. This is beneficial in providing a more robust algorithm which delivers reliable results when knowledge of the maximum frequency involved is inadequate and when modelling some complex problems.

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