

# A General-Purpose Simulator for Metamaterials with Three-Dimensional Elements

R. Mittra<sup>1,2</sup>, C. Pelletti<sup>1</sup>, R. K. Arya<sup>1</sup>, T. Dong<sup>1</sup> and G. Bianconi<sup>1</sup>

<sup>1</sup>EMC Laboratory, The Pennsylvania State University, USA

<sup>2</sup>Hi-Ci Professor, King Fahd University of Petroleum and Minerals, Dhahran - Saudi Arabia

<sup>1</sup> rajmittra@ieee.org

**Abstract**—In this paper we present two simulation techniques for modeling periodic structures with three-dimensional elements in general. The first of these is based on the Method of Moments (MoM) and is suitable for thin-wire structures, which could be either PEC or plasmonic, e.g., nanowires at optical wavelengths. The second is a Finite Difference Time Domain (FDTD)-based approach, which is well suited for handling arbitrary, inhomogeneous, three-dimensional periodic structures. Neither of the two approaches make use of the “traditional” Periodic Boundary Conditions (PBCs), and are free from the difficulties encountered in the application of the PBC, as for instance slowness in convergence (MoM) and instabilities (FDTD).

## I. INTRODUCTION

Presently, there is a considerable interest in the world of Metamaterial (MTM) and Frequency Selective Surfaces (FSSs) world in using crystals with 3D elements, because of the flexibility they provide in controlling the performance characteristic, in regard to frequency bandwidth, polarization sensitivity and angular range. An example of such an element for spatial filter is shown in Fig. 1, which achieves both a wide-angle and a wide-frequency coverage.

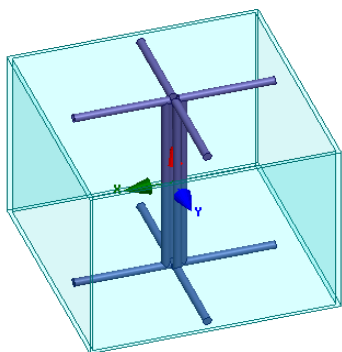


Fig. 1. Geometry of the 3D FSS unit cell

Traditionally, periodic structures are typically modeled as doubly-infinite arrays of scatterers, and are commonly analyzed, in the frequency domain, by imposing the periodic boundary condition (PBC) on a unit cell, which serves to reduce the original problem to a relatively small and manageable size [1]-[3]. The Method of Moments (MoM) [4] is typically employed for simulating FSSs with thin PEC elements, or plasmonic nanorods, by using a periodic Green's function formulation. The doubly-infinite summations in the periodic Green's function can be very time-consuming to

evaluate, and it is necessary to devise special techniques to speed up the evaluation of these summations. We show in this paper how we can handle the problem of modeling thin-rod type of periodic structures (see Fig. 2)--be they PEC or plasmonic--without the use of the periodic Green's function. Our strategy is based on two important departures from the traditional MoM techniques that use subdomain basis function for the formulation, and the periodic Green's function for the imposition of the PBC.

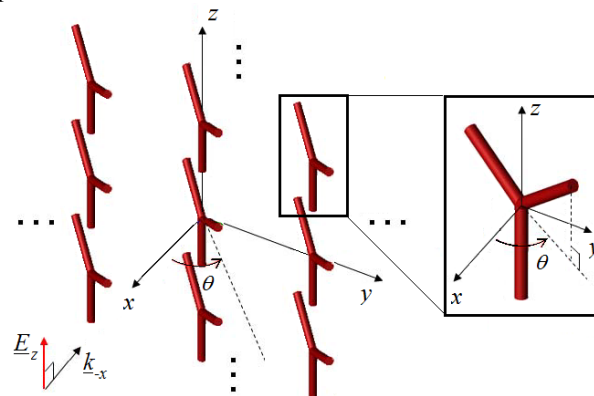


Fig. 2. Representative geometry of an infinite doubly periodic array of thin PEC tripoles tilted out-of-plane by an angle  $\theta$ .

The first step in our approach is to use the Characteristic Basis Functions (CBFs) [5] that helps reduce the number of unknowns significantly, typically to only two or three instead of hundreds. Second, we derive the results for the periodic problem at hand by extrapolating the result of a truncated version of the same which is relatively small in size, by using signal processing techniques, such as the Generalized Pencil of Function (GPOF) method [6]. We show that the proposed method achieves considerable computational efficiency, without compromising the accuracy, by bypassing the evaluation of the slowly-convergent series that arise in the evaluation of the periodic Green's function. We include some numerical examples, for rod-like elements that can be either PEC or plasmonic, to illustrate the accuracy and efficacy of the proposed approach. We do this by comparing the CPU time needed in the present approach with those required in conventional methods that utilize the PBC.

Next we turn to the problem of modeling of periodic structures with inhomogeneous and complex-shaped 3D elements (see Fig. 3). It is well known that MoM-based methods can become very inefficient when handling such

elements, and that 3D inhomogeneous FSS problem are more amenable to convenient analysis via the use of Finite Methods. We choose to use the Finite Difference Time Domain method for this purpose, because it provides us the simulation results over a wide frequency band with a single run. We note, however, that the imposition of the PBC is not very straightforward in the FDTD, which requires a modification of the update equations when dealing with periodic structures. Furthermore, FDTD is plagued by instability issues and the update algorithm requires that the time step be progressively reduced as the angle of incidence of the plane wave impinging upon the periodic structure becomes increasingly oblique.

To obviate these difficulties, we introduce yet again a technique in this paper that bypasses the use of PBCs in the FDTD. Instead, in common with the MoM-based approach described above, we again solve the problem of a truncated periodic structure to derive the solution we seek for the original periodic structure.

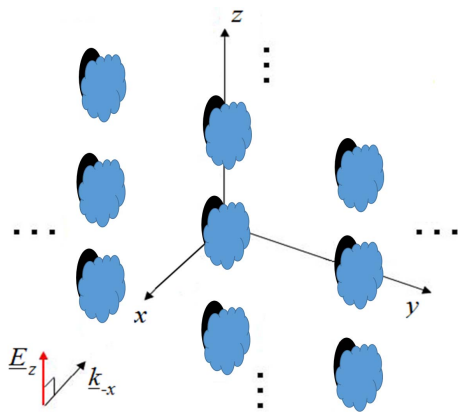


Fig. 3. Representative geometry of an infinite doubly periodic array of inhomogeneous 3D elements

Illustrative examples are also presented to demonstrate the accuracy of the approach by comparing the results derived by using an FEM-based, PBC version of the commercial code.

## II. NUMERICAL RESULTS

For the first test example, we consider a single-layer, planar, doubly-periodic FSS of infinite extent (in the  $x$ - and  $y$ -directions) with periodicities  $D_x = D_y = 0.7\lambda_0$ , where  $\lambda_0$  is the wavelength at 5 GHz. Each cell contains a PEC wire of  $\lambda_0/2$  in length, whose radius is  $\lambda_0/500$ , and which is tilted *out of plane* at an angle of  $\theta = 60^\circ$  (see Fig. 4).

An  $x$ -polarized plane wave, traveling along the  $-z$  direction, is normally incident upon the grating. Only one CBF is found to be sufficient to describe the current distribution over this type of element; hence, the related reduced matrix is just  $1 \times 1$ . The frequency range of our interest spans from 3.5 to 6 GHz.

The reflection and transmission characteristics of the array are compared in Figs. 5 and 6.

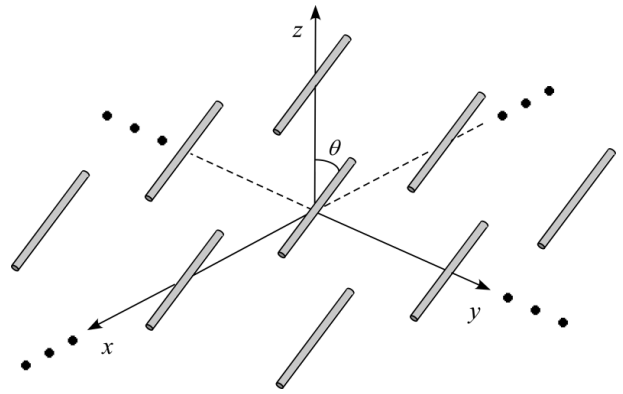


Fig. 4. Representative geometry of the analyzed periodic array of dipoles tilted out-of-plane ( $\theta = 60^\circ$ ).

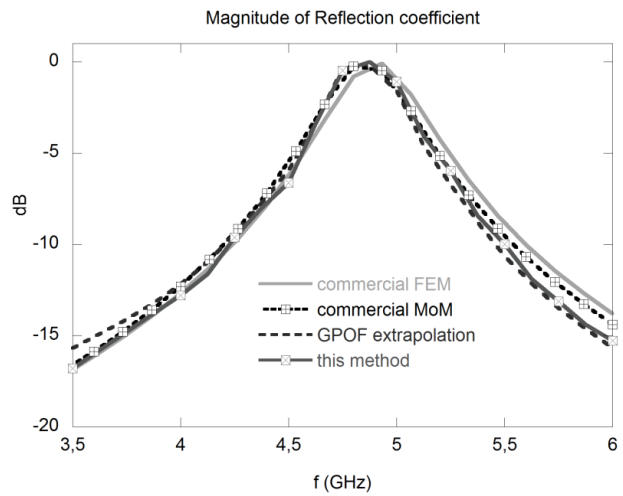


Fig. 5. Magnitude of the Reflection coefficient derived by using this method and compared with those obtained by using: GPOF extrapolation; and commercial MoM and FEM.

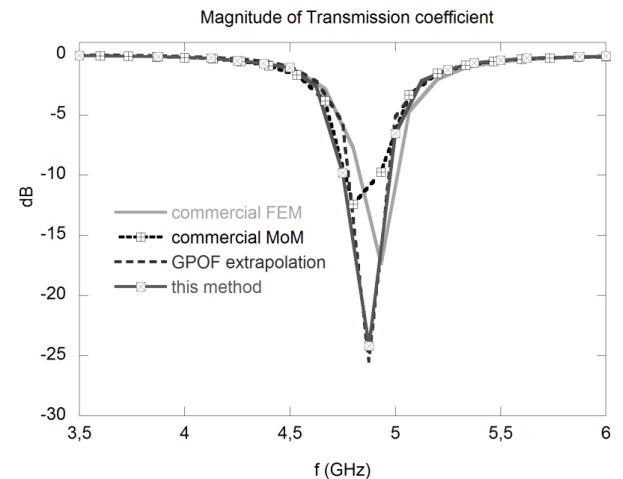


Fig. 6. Magnitude of the Transmission coefficient derived by using this method and compared with those obtained by using: GPOF extrapolation; and commercial MoM and FEM.

Table I compares the performance of the present method, in terms of run-time, against existing EM solvers and methods involving extrapolation.

TABLE I  
 RUN-TIME PERFORMANCE FOR THE DIPOLE TEST EXAMPLE BY USING THE PRESENT METHOD, GPOF EXTRAPOLATION AND COMMERCIAL SOLVERS IMPLEMENTING THE MoM AND THE FEM.

Numerical method	This method	GPOF extrapolation	MoM	FEM
Normalized time	1	9	15.5	7

For the next example, we present some representative results for the reflection characteristic of 3D structures. In Figs. 7 and 8 we show the results for an array of PEC and dielectric ( $\epsilon_r=9$ ) spheres with diameter of  $0.5\lambda_0$ , at the operating frequency of 5 GHz respectively.

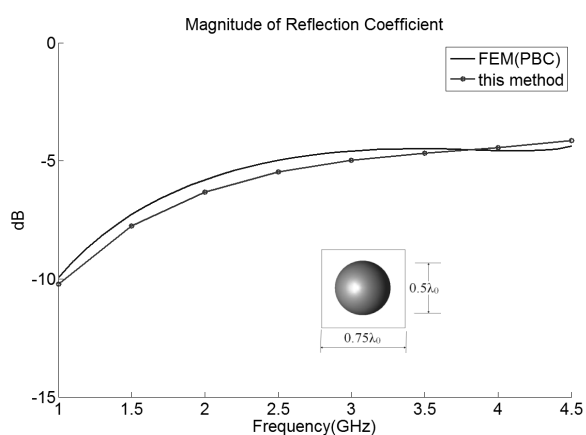


Fig. 7. Magnitude of Reflection coefficient derived by using the present method and compared with those from a commercial FEM (PBC) solver for 20 degree incidence angle for PEC spheres

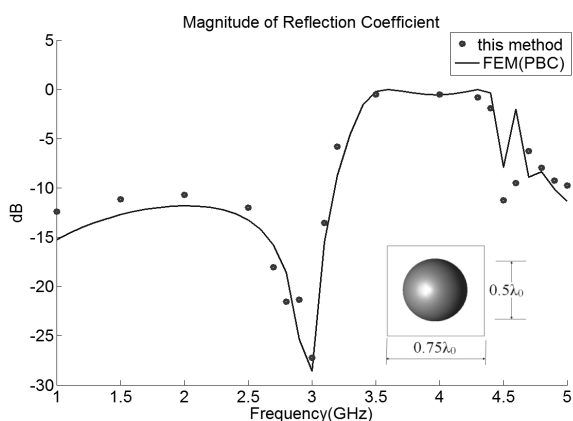


Fig. 8. Magnitude of Reflection coefficient derived by using the present method and compared with those from a commercial FEM (PBC) solver for 20 degree incidence angle for dielectric spheres

### III. CONCLUSION

In this paper, we have introduced two simulation techniques for modelling periodic structures with three-dimensional elements. The proposed first technique yields accurate results for the reflection and transmission characteristics of the array, at a fraction of the computational cost when compared to those required by existing codes for modeling periodic structures. The computational efficiency is realized by totally bypassing the evaluation of the infinite summations, either in the spatial or in the spectral domains. Also, we have introduced second technique to derive the response characteristics of periodic arrays characterized by arbitrary 3D type of elements. This method yields results that are in good agreement with those obtained from commercial solvers, while it avoids the use of PBCs, thus bypassing the difficulties encountered in the FDTD with the increase in the solve-time, and with issues pertaining to the stability behavior.

Before closing, we mention that the techniques presented herein can be modified to address the important problem of modeling periodic structures with statistical variations in their geometries, as is typically case with MTMs for optical wavelengths, where the difficulties in their fabrication almost always introduce small variations in the dimensions of the elements that comprise the "periodic" array.

### REFERENCES

- [1] Mittra, R., C. H. Chan and T. Cwik, "Techniques for Analyzing Frequency Selective Surfaces-a Review," *IEEE Proc.*, Vol. 76, No. 12, 1593-1615, 1988.
- [2] B.A. Munk, *Frequency selective surfaces: Theory and design*, Wiley, New York, 2000.
- [3] A. Taflov and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed. Norwood, MA: Artech House, 2005.
- [4] R. F. Harrington, *Field Computation by Moment Method*, New York: The Macmillan Company, 1968.
- [5] V.V.S. Prakash, R. Mittra, "Characteristic basis function method: A new technique for efficient solution of method of moments matrix equations," *Microwave and Optical Technology Letters*, Vol. 36, No. 2, pp. 95-100, Jan. 2003.
- [6] Y. Hua, T. Sarkar, "Generalized Pencil-of-Functions Method for Extracting Poles of an EM System from Its Transient Response," *IEEE Trans. Antennas and Propag.*, Vol. 37, No. 2, pp. 229-234, Feb. 1989.