

# Numerical Methods for Analyzing Periodic Metamaterials

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## Abstract

We present a variety of numerical techniques to model metamaterial geometries involving periodic structures of infinite or finite size. Accelerated method of moments and FDTD techniques are used to model metamaterials with infinite extent in one or more dimensions that are excited by either periodic excitations or by a localized (non-periodic) source. Fast solvers like GIFFT (Green's function Interpolation and FFT) and as well as techniques such as the use of macro basis functions are used to model metamaterials having a large finite size.

## 1. Introduction

Due to the recent explosion of interest in studying the electromagnetic behavior of periodic structures such as metamaterials, metasurfaces, and photonic crystals, there has been a renewed effort to efficiently model such structures. This includes estimating transmission and reflection properties of metamaterials illuminated by plane waves, determining the dispersion characteristics for modal propagation in these periodic structures, calculating the fields from single (non-periodic) sources near infinite periodic metamaterial structures, and modeling metamaterials of finite size. Since straightforward numerical analyses of large, finite periodic structures (i.e., explicitly meshing and computing interactions between all elements of the entire structure) involves significant memory storage and computation time, much effort is currently being expended on developing techniques that minimize the computational resources.

In this presentation we will summarize our recent efforts in modeling infinite and finite periodic structures by exploring a few complementary numerical techniques in the frequency domain and in the time domain. Numerical results will be presented to demonstrate the applicability and the numerical efficiency of these various techniques for a wide variety of structures, with applications ranging from microwave EBG structures to photonic structures at optical frequencies.

Table 1 below as well as references [1]-[11] summarize the various numerical possibilities we have been working on to model both infinite and large but finite (periodic and non-periodic) metamaterials.

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## 2. Summary of numerical techniques

### 2.a. Metamaterials with infinite extent

We have derived accelerated periodic Green's functions (GFs) by using the Ewald method for 3D elements with periodicity in 2D [1] and 1D [2], and for 2D elements with periodicity in 1D [3]. The computation of these accelerated Green's requires the evaluation of only a handful of terms. They are used to model dispersion characteristics as well as calculate the fields from sources in multilayer environments [4]-[5]. In particular, complex modes in periodic structures pose some challenges due to the increased complexity of the spectral wavenumber plane; some examples will be presented.

Also, the FDTD method can be efficiently used to model periodic structures when special spectral boundary conditions (BC) are used, consisting of a phase shift condition applied in the time domain (therefore dealing with complex time-domain quantities) [6].

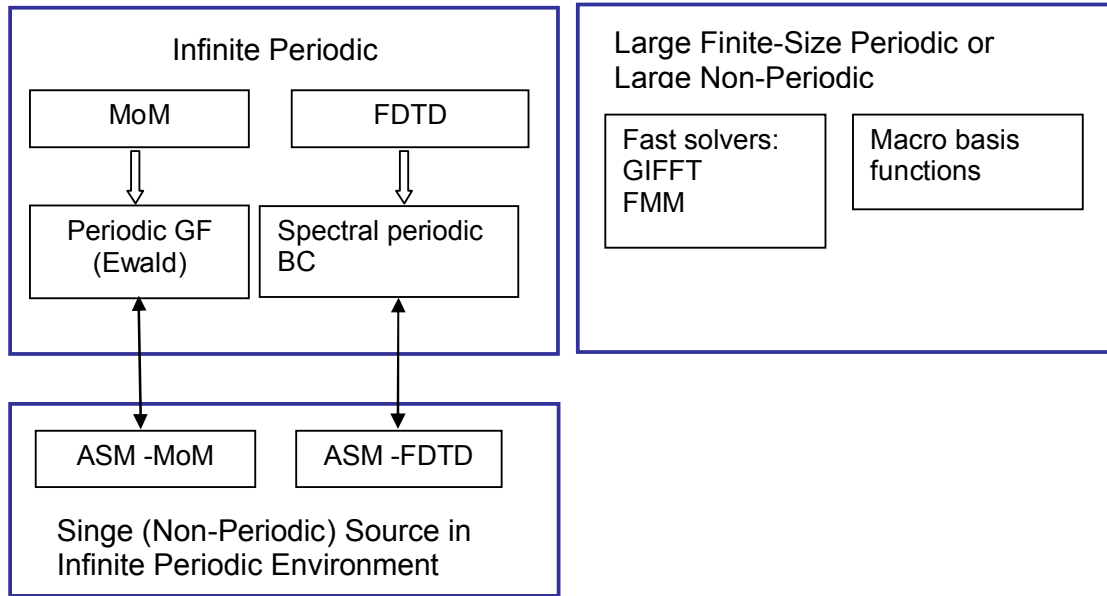
The periodic GF analyses in the frequency and time domains can be used in conjunction with the array scanning method (ASM) to model finite non-periodic sources in the presence of infinite periodic structures [7]-[8]. We will show some of the analytic properties of the field produced by a source in the presence of an infinite periodic structure, and we will discuss two algorithms, one in the frequency domain (ASM-MoM) and the other in the time domain (ASM-FDTD) [9], together with several applications. In either ASM-MoM or ASM-FDTD, the field of the source in the presence of the infinite periodic structure is calculated by numerical simulation of only a *single unit cell*. This allows for tremendous memory savings (and usually savings in calculation time as well) compared with a "brute-force" numerical simulation in which the infinite periodic structure is approximated numerically by simulating many unit cells.

### 2.b. Metamaterials with finite extent

Large periodic structures of finite size can be modeled with fast solvers; in particular we have recently developed the method called GIFFT (Green's function Interpolation and FFT) which dramatically reduces the number of GF calculations needed in the solution process as well as the matrix setup time and solve time when modeling this class of structures [10]-[11]. One of the advantages of this method compared to other fast solvers such as the Fast Multipole Method (FMM) is that, because GIFFT uses relatively sparse samples of the GF in the spatial domain, it is very beneficial for layered-media environments, which involve a rather time-consuming Green's function calculation. In this method the Green's function is interpolated in a separable form (with respect to the source and observation points) on a fairly sparse grid. This allows for many fewer calculations of the time-consuming layered-media Green's function, and also (because of the separable form) allows for the use of the FFT when calculating the basis-testing interactions that are needed in the matrix fill. We will show the performance of this method and some applications for modeling metamaterials. With the GIFFT method metamaterial problems that would require hundred of thousands of unknowns with the standard MoM can be simulated with personal computers. The GIFFT method is ideal for large finite periodic structures where each periodic element requires a large number of unknowns.

An alternative fast technique consists in reducing dramatically the number of unknowns through a compact description of the current (or field when modeling dielectrics) over the unit cell. This may be obtained through the solution of small finite periodic problems, or through a specific use of infinite array solutions (from which eigenmodes can be obtained) as well as field distributions in the presence of non-periodic excitations. Those solutions can then be used as macro (or characteristic) basis functions [12]. Specific methods also have been developed to obtain the interaction between these global basis functions.

**Table 1.** Diagram showing various numerical techniques that are considered here for the efficient modeling of periodic metamaterials having infinite or finite extent.



## References

1. S. Oroskar, D. R. Jackson and D. R. Wilton, "Efficient computation of the 2D periodic Green's function using the Ewald method," *Journal of Comp. Physics*, Volume 219, Issue 2, pp 899-911, 10 Dec. 2006.
2. F. Capolino, D. R. Wilton, W. A. Johnson, "Efficient Computation of the 3D Green's Function for the Helmholtz Operator for a linear Array of Point Sources Using the Ewald Method," *Journal of Computational Physics*, on line since Nov. 2006. doi:10.1016/j.jcp.2006.09.013, vol. 223, pp. 250-261, April 2007.
3. F. Capolino, D. R. Wilton and W. A. Johnson, "Efficient Computation of the 2-D Green's Function for 1-D Periodic Arrays Using the Ewald Method," *IEEE Trans. Antennas and Propagation*, Vol. 53, N.9, pp. 2977-2984, Sept. 2005.
4. W. A. Johnson, L. I. Babilio, J. D. Kotulski, R. E. Jorgenson, L. K. Warne, R. S. Coats, D. R. Wilton, N. J. Champagne, F. Capolino, J. B. Grant, and M. A. Khayat, "EIGER an Open Source Frequency Domain Electromagnetics Code," *IEEE APS-Symp.* Honolulu, Hawaii, USA, 10-15 June 2007.
5. D. R. Jackson, D. R. Wilton, N. J. Champagne, "Efficient computation of periodic and nonperiodic Green's function in layered media using the MPIE," *URSI Int. Symp. on Electrom. Theory*, Thessaloniki, Greece, May 25-28, 1998.
6. F. Yang, J. Chen, R. Qiang, and A. Elsherbeni, "FDTD analysis of periodic structures at arbitrary incidence angles: a simple and efficient implementation of the periodic boundary conditions", *IEEE Antennas and Propagation Society Intern Symp.*, pp. 2715-2718, Albuquerque, NM, June 2006.

7. F. Capolino, D. R. Jackson and D. R. Wilton, "Fundamental Properties of the Field at the Interface Between Air and a Periodic Artificial Material Excited by a Line Source," *IEEE Trans. Antennas and Propagat.*, Special Issue on Artificial Magnetic Conductors, Soft/Hard Surfaces, and Other Complex Surfaces, Vol.53, N.1, pp.91-99, Jan. 2005.
8. F. Capolino, D. R. Jackson, D. R. Wilton, and L. B. Felsen, "Comparison of methods for calculating the field excited by a dipole near a 2-D periodic material," *IEEE Trans. Antennas and Propagat.*, vol. 55, No.6, Part I, pp. 1644-1655, June 2007.
9. R. Qiang, J. Chen, F. Capolino, D. R. Jackson, and D. R. Wilton, "Array Scanning Method-FDTD for Emission of Finite Electromagnetic Sources in Periodic Artificial Materials," *IEEE Microwave on Wireless Components Letters*, vol. 17, no. 4, pp. 271-273, April 2007
10. B. J. Fassenfest, F. Capolino, D. R. Wilton, and D. R. Jackson, N. Champagne, "A Fast MoM Solution for Large Arrays: Green's Function Interpolation with FFT," *IEEE Antennas and Wireless Propagat. Letters*, Vol. 3, pp. 161-164, 2004.
11. B. J. Fassenfest, F. Capolino, and D. R. Wilton, "Preconditioned GIFFT: A Fast MoM Solver for Large Arrays of Printed Antennas," *Invited paper - Journal ACES (Applied Computational Electromagnetic Society), Special Issue on Arrays*, Vol. 21, N. 3, pp. 276-283, Nov. 2006.
12. C. Craeye, Th. Gilles, Combination of multipole and macro basis function approaches for the analysis of finite arrays with dielectric elements, *Proc. of the First European Conference on Antennas and Propagation (EUCAP)*, Nice, France, Nov. 2006.
13. C. Craeye and F. Capolino, "Accelerated Computation of the Free Space Green's Function of Semi-Infinite Phased Arrays of dipoles," *IEEE Trans. Antennas and Propagation*, Vol. 54, N.3, pp.1037-1040, Mar. 2006.