Advances in Time-Domain Modeling of Periodic Structures and Related Metamaterial Applications

C. D. Sarris*

Abstract — The periodic analysis of candidate plasmonic topologies for the implementation of left-handed media at optical frequencies is pursued through a triangular mesh based Finite-Difference Time-Domain (FDTD), equipped with Floquet boundary conditions. The technique is shown to possess excellent convergence and accuracy properties, as opposed to the conventional rectangular cell based FDTD.

1 INTRODUCTION

It is widely recognized that Veselago’s early work on the possibility of media concurrently exhibiting negative dielectric permittivity $\varepsilon$ and magnetic permeability $\mu$ [1] has been the main inspiration for the recent activity in the area of metamaterials. Veselago introduced the term left-handed for such media after the formation of a left-handed triplet by the electric, magnetic and wave vectors in those and suggested that the index of refraction in left-handed media would be negative. The theoretical results of [1] were experimentally confirmed through microwave artificial dielectrics exhibiting negative refractive index (NRI), with the split-ring resonator and strip wire (SRR/SW) structure of [2] being the first realization of such. A planar alternative, exhibiting a wide NRI bandwidth compared to the strongly resonant SRR/SW geometry, was proposed in [3]. The latter was based on a two-dimensional transmission-line (TL) loaded by lumped elements. Therefore, the extension of the NRI-TL concept to optical frequencies, while appealing due to its potential for broad bandwidth, becomes synonymous with the conception of optical analogs of lumped elements.

Recently, Engheta et al. addressed this question by identifying lattices of plasmonic spheres/ellipsoids as possible counterparts of the NRI-TL structure in the infrared and visible regime [4]. Furthermore, one and two-dimensional arrays of silver nanoparticles have been shown to exhibit backward-wave bands, the signature property of NRI media, within their Brillouin zone [5]. In this paper, the dispersion analysis of periodic structures of plasmonic rods is performed through the Finite-Difference Time-Domain (FDTD) technique [6]. FDTD is simple, versatile and provides for the wideband characterization of geometries in a single simulation. However, its cartesian mesh version would approximate a cylindrical or spherical inclusion by mesh stair-casing. In principle, the well-known numerical errors due to stair-casing [7] can be reduced by mesh refinement of the standard FDTD or by modified FDTD schemes aimed at improving the modeling of non-rectangular boundaries [8]. The studies included here show that these errors become quite pronounced when plasmonic modes are involved, resulting in spurious resonances. In the following, our approach to the FDTD dispersion analysis of two-dimensional arrays of plasmonic nanoparticles is presented, along with a comparison to the conventional rectangular mesh FDTD. Subsequently, the proposed methodology is employed for the calculation of the complete band diagram of the SPC of [5], providing a solid background for the understanding of its operation, including its narrowband behavior as a lens.

2 TRIANGULAR MESH PERIODIC FDTD

2.1 Update Equations

A two-dimensional transverse electric (2D-TE) case is considered, with $E_x$, $E_y$, and $H_z$ field components. The computational domain is divided in triangular elements, generated by a Delauny triangular mesh generator. In each element, tangential electric field components are sampled at the center of each edge and the perpendicular magnetic field component is sampled at a “centroid” point, whose coordinates are computed by averaging the coordinates of the triangle vertices.

Recently, Engheta et al. addressed this question by identifying lattices of plasmonic spheres/ellipsoids as possible counterparts of the NRI-TL structure in the infrared and visible regime [4]. Furthermore, one and two-dimensional arrays of silver nanoparticles have been shown to exhibit backward-wave bands, the signature property of NRI media, within their Brillouin zone [5]. In this paper, the dispersion analysis of periodic structures of plasmonic rods is performed through the Finite-Difference Time-Domain (FDTD) technique [6]. FDTD is simple, versatile and provides for the wideband characterization of geometries in a single simulation. However, its cartesian mesh version would approximate a cylindrical or spherical inclusion by mesh stair-casing. In principle, the well-known numerical errors due to stair-casing [7] can be reduced by mesh refinement of the standard FDTD or by modified FDTD schemes aimed at improving the modeling of non-rectangular boundaries [8]. The studies included here show that these errors become quite pronounced when plasmonic modes are involved, resulting in spurious resonances. In the following, our approach to the FDTD dispersion analysis of two-dimensional arrays of plasmonic nanoparticles is presented, along with a comparison to the conventional rectangular mesh FDTD. Subsequently, the proposed methodology is employed for the calculation of the complete band diagram of the SPC of [5], providing a solid background for the understanding of its operation, including its narrowband behavior as a lens.

$$\frac{\partial H_z}{\partial t} A \approx E_1|P_2P_3| + E_2|P_3P_1| + E_3|P_1P_2| \quad (1)$$
Approximating the remaining time derivative by a second order accurate centered difference, the following update equation is derived:

\[ H_{z}^{n+1/2} = H_{z}^{n-1/2} + \frac{\Delta t}{\mu A} \left( E_{t1}^{n} \left| P_2P_3 \right| + E_{t3}^{n} \left| P_1P_2 \right| \right) \]

\[ + E_{t2}^{n} \left| P_3P_1 \right| + E_{t3}^{n} \left| P_1P_2 \right| \]

where \( \Delta t \) is the time step and \( n \) is a time-step index. Similarly, the update equation for the tangential electric field components stems from the application of Ampere’s law, using the line segment connecting the centroids of two adjacent triangles, shown in Fig. 1, as an Amperian path:

\[ \frac{\partial D_{t}}{\partial t} \left| Q_1Q_2 \right| \sin \tau \approx H_{z1}^{n+1/2} - H_{z2}^{n+1/2} \]

Hence, the update equation for a tangential electric flux density component \( D_{t} \) assumes the form:

\[ D_{t}^{n+1} = D_{t}^{n} + \frac{\Delta t}{\left| Q_1Q_2 \right| \sin \tau} \left( H_{z1} - H_{z2} \right) \]

The incorporation of the material dispersion characterizing the plasmonic nanoparticles is performed by translating the frequency-domain constitutive relation \( \bar{D}_{t}(\omega) = \bar{\epsilon}(\omega) \bar{E}_{t}(\omega) \) (where \( \bar{\cdot} \) denotes a phasor quantity) to the time-domain. To that end, an auxiliary differential equation method, associating the dispersive dielectric permittivity to a polarization current, as detailed in [6], is employed. For the dielectric permittivity \( \epsilon(\omega) \), the Drude model is used, assuming an \( e^{\sigma t} \) time-dependence: \( \epsilon(\omega) = 1 - \left( \omega_{p}/\omega \right)^{2} \).

2.2 Implementation of Periodic Boundary Conditions

In a two-dimensional periodic structure of spatial period \( d_{x} \) and \( d_{y} \) along the \( x \)- and \( y \)-axes of a rectangular coordinate system, phasor field components one period away in either direction differ only by a constant attenuation and phase shift term \( e^{-jk_{x}d_{x}} \), \( e^{-jk_{y}d_{y}} \) respectively, where \( \mathbf{k} = \hat{x}k_{x} + \hat{y}k_{y} \) is a Bloch wavevector. This frequency-domain relationship is translated into the time-domain via the sine-cosine method of [9]. The following considerations are specifically pertinent to the implementation of periodic boundaries in the triangular FDTD mesh. Consider, for example, a wave propagating along the \( y \)-axis, with a Bloch wavevector \( \mathbf{k} = \hat{y}k_{y} \), in a periodic structure of the unit cell shown in Fig. 2. Note that although the magnetic field node \( H_{z,b} \) is outside the unit cell, it is connected to the magnetic field node \( H_{z,a} \) at a distance \( d_{y} \) along the \( y \)-axis inside the cell, through the periodic boundary condition:

\[ \bar{H}_{z,b} = \bar{H}_{z,a} e^{-j k_{y} d_{y}} \]

Then, the tangential electric field component along \( DF \) can be updated, according to the stencil of Fig. 1. However, the triangle enclosing the \( H_{z,b} \) node has to be the same as the one enclosing the \( H_{z,a} \) node, for the two periodic boundaries to be identical, not just physically but numerically as well. Therefore, the triangle \( DFG \) is generated by translating \( ABC \) by \( d_{y} \) along the \( y \)-axis. Evidently, the segmentation of the periodic boundaries is also identical; if the left boundary \( (y = 0) \) is divided in segments \( P_1P_2 \cdots P_N \) and the right boundary \( (y = d_{y}) \) is divided in segments \( Q_1Q_2 \cdots Q_N \), then: \( |P_{i}P_{i+1}| = |Q_{i}Q_{i+1}|, i = 1, 2, \cdots, N - 1 \). Similarly, the discretization of the lower and upper boundaries is identical. Finally, modal field distributions can be obtained by Fourier transforming sampled field values over a mesh of points.

3 PERIODIC ANALYSIS OF THE SPC LATTICE

3.1 Numerical Results: Rectangular and Triangular Mesh FDTD

One of the motivating applications of this work, namely the SPC lattice of [5], is considered next.
The specifications of the geometry, shown in Fig. 3, are normalized to the plasma frequency of the silver rods; the lattice period is $a = c/\omega_p$ and the radius of the cylinders is $r = 0.45a$. The SPC lattice was modeled in [5] by both quasi-static and full-wave (finite element) means. On the other hand, the triangular FDTD technique is employed here for the periodic analysis of the same structure. The periodic analysis results derived by the triangular mesh FDTD are summarized in Fig. 4, which compares the present analysis to the one of [5] (which provided the $\Gamma - X$ part of the Brillouin diagram of the SPC lattice). While the modes predicted by the analysis of [5] have been also found here, two additional ones have been extracted as well. Only the third of these modes is backward due to its slightly negative group velocity. This mode was used in [5] to realize a "perfect lens". However, since this mode is closely surrounded by forward ones, the lensing effect cannot be maintained over a practically significant bandwidth.

To obtain more clear insights to the usefulness of the proposed formulation, results deduced via the conventional rectangular mesh FDTD, for frequencies up to $0.7\omega_p$, are presented first. In particular, Figs. 5 (a), (b) depict the Fourier transform of $H_z$ sampled inside the unit cell of the SPC lattice, for several Bloch wavevectors $\vec{k} = \hat{x}k_x$ (along $\Gamma - X$). Although clear resonances can be seen up to $0.38\omega_p$, higher frequency resonances present a noise-like rather than resonant pattern. In addition, convergence of the resonant frequency peaks that appear above $0.38\omega_p$ cannot be achieved by mesh refinement. On the other hand, the triangular mesh FDTD allows for a quickly convergent calculation of these resonant frequencies even at a relatively coarse mesh (Fig. 5 (c), (d)).

4 CONCLUSIONS

A simple, explicit and stable formulation of the FDTD technique, employing a triangular mesh, has been shown to be a well convergent, efficient tool for the periodic analysis of two-dimensional arrays of plasmonic nanorods, possibly useful for optical implementations of NRI media. However, the analysis of the interaction of such structures with non-periodic sources cannot be performed within the same framework. This problem is addressed through the coupling of the well-known array scanning method with the sine-cosine technique [10].

Acknowledgments

This work is the product of a fruitful collaboration of the author with Dr. Y. Liu, D. Li, and Prof. G.V. Eleftheriades. Research support has been provided by the Natural Sciences and Engineering Re-
 References


Figure 5: Power spectral density of \( H_z \), deduced by a rectangular mesh FDTD and the proposed method for various sizes of Yee cells/minimum sizes of triangle edges and Bloch wavevectors \( \vec{k} = \pm k_z \). Legends indicate \( k_z/a \) values, where \( a \) is the lattice period.