A Generalized Subcell Method for FDTD

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Many structures of recent interest in metamaterial and metasurface studies consist of periodic arrangements of unit cells with deeply subwavelength features (A. Epstein, G.V. Eleftheriades, *J. Opt. Soc. Am. B*, vol. 33, no. 2, 2016). For discrete space-time methods, such as the Finite-Difference Time-Domain (FDTD), these cases are doubly problematic, as the necessary mesh refinement is accompanied by a reduction in the maximum allowable time step, dictated by the Courant-Friedrichs-Lewy stability condition. This problem is typically dealt with with local mesh refinement, either realized with a non-uniform mesh or a subgrid. Both methods result in deeply subwavelength cells, sampling the desired solution to the problem at hand at a sampling rate that significantly surpasses the Nyquist limit.

Alternatively, thin layer, subcell (G. Maloney, G. S. Smith, *IEEE Trans. Antennas Propagat.*, vol. 40, no. 3, Mar. 1992) and surface impedance boundary condition methods (M. K. Kärkkäinen, *IEEE Trans. Antennas Propagat.*, vol. 46, no. 2, May 2004) can be used, locally modifying a standard FDTD scheme. However, all of these methods treat canonical cases of thin layers, generally aligned with one of the three axes of the cell, which extend over one whole cell in two of the three dimensions and cover a portion of the cell in the third. Therefore, these techniques lack the flexibility of subgrids, in the sense that they cannot deal with arbitrarily shaped subwavelength features embedded in a Yee cell.

We formulate and apply a generalized method that allows for embedding arbitrarily shaped, electrically small features in a single Yee cell. For each cell we derive tensor effective parameters by a partial filled capacitor/inductor method: terminating the cell in two parallel plates in the $x-$, $y-$ and $z-$ directions and extracting the corresponding effective permittivity and permeability from the capacitance/inductance of the parallel plate capacitor/inductor formed by the plates and the cell. Then, the standard FDTD update equations remain structurally unaltered, yet they incorporate the tensor effective parameters that account for the presence of subcellular features.

A detailed accuracy analysis is performed to illustrate the potential and the limitations of this approach, followed by applications of metasurfaces with metallic, dielectric, conducting and dispersive subwavelength, three-dimensional subcell features. Special emphasis is given to modeling subcell graphene inclusions.