# Parallel Finite Difference Time Domain Codes for Electromagnetic Metamaterial Calculations

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*Abstract*— **A set of freely available Parallel Finite Difference Time Domain codes for distributed memory platforms are presented to simulate the propagation of electromagnetic waves in metamaterials and photonic crystals. The FDTD algorithms are supplemented with metamaterial homogenization procedures. The effective permittivity and magnetic permeability of metamaterials are calculate in two different ways, with direct homogenization of the fields over the periodic cell of the metamaterial and extracted from transmission reflection data. The algorithms are applied to extract the effective material parameters of multilayer fishnet metamaterials and to demonstrate the focusing effect of dielectric rods under plane wave illumination.**

*Index Terms*—**Metamaterials, Electromagnetic propagation, Finite difference methods, Effective material parameters.**

## I. INTRODUCTION

Metamaterials are electromagnetic structures receiving their novel and unusual properties from micro- or nanostructuring of materials instead of chemical composition [1]. Usually metamaterials are periodic structures of metals and dielectrics with subwavelength features. In order to understand the interaction of electromagnetic waves with metamaterials, and to design new metamaterial based devices, the precise solution of Maxwell's equations is essential. A large number of commercial and freely available numerical solvers are available for Maxwell's equations; however the simulation of metallic structures with subwavelength features presents specific challenges. Nanostructures, especially those made of metals, can have resonances with very high quality factor and at the same time they can concentrate the electromagnetic energy in very small volumes. The Finite Difference Time Domain (FDTD) method [2] is a powerful iterative numerical technique to solve the Maxwell equations. A distinct advantage of the method is that it can be easily parallelized. Therefore the FDTD method is an optimal choice to accurately simulate metamaterials on parallel platforms with distributed memory architectures.

Based on the FDTD method parallel object oriented C++ codes have been developed to simulate the propagation of electromagnetic waves in metamaterials and photonic crystals. The algorithms are supplemented with effective parameter extraction and homogenization procedures in order to calculate the effective electric permittivity and magnetic permeability of metamaterials. Two examples demonstrate the features of the developed software. The first example presents the extraction of effective material parameters of a multilayer fishnet metamaterial. The second example demonstrates the focusing effect of dielectric rods under plane wave illumination.

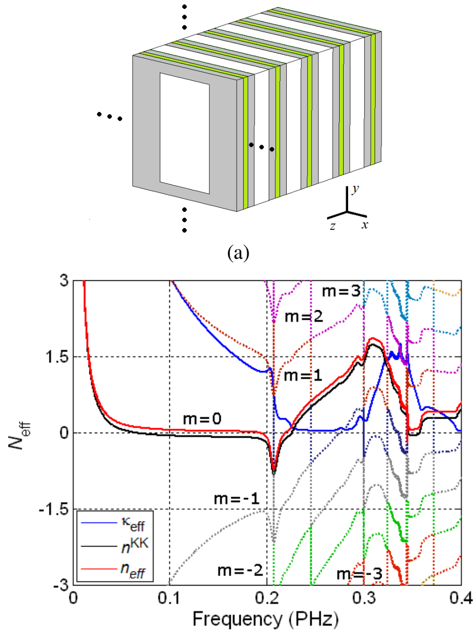
## II. PARALLEL FDTD CODES FOR MIXED COMPUTING PLATFORM

It is a difficult task to develop a software, which performs evenly well on diverse parallel architectures. Therefore the developed FDTD algorithm has two levels of parallelization. The first level explores the distributed memory architectures. The computational volume is divided into sub volumes according to the nodes of the system. A process is started for every sub volume to perform the FDTD calculations. The Message Passing Interface is used to communicate between processes the electromagnetic field values required at the sides of sub-volume. The second level of parallelization, which is implemented with OpenMp directives, explores the advantages of shared memory space inside of one node with the nowadays common multi-core processors. The computational space can be truncated with Uniaxial Perfectly Matched Layer or periodic boundary conditions. The software supports point sources or plane wave excitation with the Total Field–Scattered Field formulation. The polarization and propagation direction of the plane waves can be arbitrary. Constant material parameters and dispersive electric permittivity with arbitrary number of Lorentz terms are supported. The developed codes have been published online and are freely available [3]. The software can be run under UNIX and Windows operating system as well.

## III. HOMOGENIZATION AND EFFECTIVE METAMATERIAL PARAMETER EXTRACTION

Metamaterials and photonic crystals are periodic structures, which are often utilized in form of slabs. The developed FDTD codes can handle periodic boundary conditions, in two spatial dimensions and absorbing boundary condition in the third direction, which makes possible the efficient simulation of transmission reflection data and of the electromagnetic field distribution of structured slabs. The transmission reflection data and the distribution of the electromagnetic fields makes possible to homogenize metamaterials in two distinct ways.

The effective metamaterial parameters can be extracted by replacing the electromagnetic response of the complicated metamaterial structure with the electromagnetic response of a homogeneous slab. From the Fresnel relations, who express the transmission and reflection of homogeneous slabs in function of material parameters, the wave impedance and the refractive index can be calculated. However, the calculation of the refractive index involves the evaluation of a complex logarithm that is a multi-valued function. The resulting uncertainty is referred to as branching problem, which affects only the real part of the refractive index. To remove this ambiguity, the Kramers-Kronig relation can be applied to estimate the refractive index from the extinction coefficient [4]. The physically realistic exact values of the refractive index are determined by selecting those branches of the logarithmic function which are closest to those predicted by the Kramers-Kronig relation. Fig. 1 presents the geometry and the extracted effective refractive index of the multilayer fishnet. The dimensions and the material parameters of individual fishnet layers (Ag-$MgF_2$-Ag) are the same as in [5]. The separation distance between the fishnet layers is 100 nm.



(a)

(b)

Fig. 1. Homogenization of the multilayer fishnet structure. In (a) the geometry of the metamaterial built of five fishnet layers is presented. In (b) the calculated extinction coefficient $\kappa_{eff}$, the refractive index obtained from the Kramers-Kronig relation $n^{KK}$, several possible branches of the refractive index and the unambiguously retrieved refractive index $n_{eff}$ are presented.

The calculation of the effective parameters of metamaterial slabs with field averaging is a cumbersome problem and has to date not been entirely resolved. The implemented dynamic effective medium theory relates the Fourier components of the fields with the effective electric permittivity and magnetic permeability at one magnitude of the wave vector, which is the propagating mode [6]

$$\int_V \mathbf{D}(\mathbf{r},\omega)e^{ik_{eff}z}d\mathbf{r}=\varepsilon_{eff}\int_V \mathbf{E}(\mathbf{r},\omega)e^{ik_{eff}z}d\mathbf{r},$$

$$\int_V B(\mathbf{r},\omega)e^{ik_{eff}z}d\mathbf{r}=\mu_{eff}\int_V \mathbf{H}(\mathbf{r},\omega)e^{ik_{eff}z}d\mathbf{r},$$

where the wave number of the propagating mode is $k_{eff}=\sqrt{\varepsilon_{eff}\mu_{eff}}\,\omega/c$ and the volume of integration $V$ is usually chosen arbitrarily. For thick metamaterial slabs it may correspond to the volume of the unit cells away from the boundaries, while for thin slabs it may be the full volume of the metamaterial. The developed open source FDTD software allows straightforward implementation of other field averaging methods as well [7].

## IV. FOCUSING EFFECT OF DIELECTRIC NANORODS

The developed FDTD codes have been applied to investigate the electromagnetic field propagation through focusing nanorods [8], see Fig. 2, where the high intensity spot occur at a distance of several wavelengths away from the structure. The simulations demonstrate that the focusing effect is maintained even when nanorods are missing from the structure due to fabrication errors.

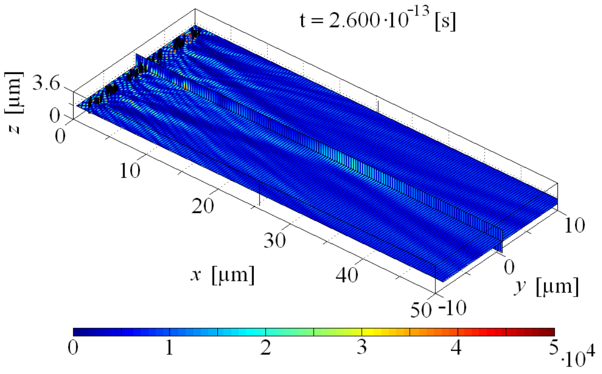


Fig. 2. The intensity distribution of the focusing nanorods.

## V. CONCLUSIONS

Freely available software package of parallel FDTD codes has been presented with the hope that they are useful for scientist working in the research field of metamaterials and in a wider sense for people interested in computational electrodynamics.

## ACKNOWLEDGEMENT

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