Efficient Calculation of Effective Material Parameters in Metamaterials Using FDTD and a Modal Approach

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Abstract — **We present an efficient modal approach in combination with the Finite Integration Technique (FIT) – a generalized FDTD-like method – to analyze resonant structures. Rather than performing time-consuming time-stepping of long transients, the eigenmodes of the spatial discretization operators are utilized to extract frequency-domain parameters of the simulated devices. As an application we calculate averaged material parameters of recently proposed so-called metamaterials, which show a distinctive resonant behavior with negative permittivity and permeability in a certain frequency range.**

I. Introduction

Grid-based simulation methods like the Finite Difference Time Domain (FDTD) method, Finite Element (FE) approaches or the Finite Integration Technique (FIT) – the latter is used in this paper – are powerful tools for the analysis of microwave devices. This is especially true for time domain approaches, where broadband results e.g. for the scattering parameters can be obtained by a single simulation run with appropriate input signals.

However, new problems arise with the simulation of *highly resonant* devices, where, due to the long settling times, the time domain approach requires a large number of time steps to reach steady state. If the goal of the simulation is a precise prediction of the system's response near a resonance, the use of approximate techniques, such as introducing artificial losses or non-conservative time integration schemes, is not acceptable. On the other hand, a conventional eigenvalue analysis (in frequency domain) of the 'closed' structure, with short circuits at the input/output ports, only gives a hint on the resonance frequencies, but no quantitative results for the behavior of the original (open) device around that frequency.

One example of such a resonant structure, which will be dealt with in this paper, is the calculation of averaged material coefficients in so-called metamaterials [1,2,3]. Metamaterials consist of a lattice of conducting, nonmagnetic elements that can be described by an effective magnetic permeability μ_{eff} and an effective electrical permittivity ε_{eff}, both of which can exhibit values not found in naturally occurring materials. Typically each cell of the lattice represents a resonant structure with spatial dimensions much smaller than the incident wavelength. The effective material parameters can then be defined as the ratios of averaged field and flux quantities over one cell [1]. The task for the numerical simulation is to extract these parameters from the electromagnetic fields over a certain frequency range.

For the analysis of these resonant structures we present here an efficient *modal approach*, which was previously used for the calculation of scattering parameters in [4]. This method is based on an incomplete eigenvalue decomposition of the *spatial* system matrix, and no time-stepping has to be performed. As underlying discretization scheme we use the Finite Integration Technique (FIT), which can be considered as a generalized finite difference method and which has close relations to the well-known FDTD-method.

II. The Finite Integration Technique (FIT)

A. Basics and Notation of FIT

Similar to the FDTD method, the Finite Integration Technique [5,6] uses a pair of staggered grids, the primary grid G and the dual grid $\tilde{G}$, which however can have a more general structure as the standard "Yee cell" of FDTD. The state variables of FIT are so-called grid voltages and grid fluxes which are defined as *integrals* of the electric and magnetic fields on edges L_i, $\tilde{L}_i$ or faces A_i, $\tilde{A}_i$ of G and $\tilde{G}$, respectively:

$$\begin{aligned} \hat{e}_i &= \int_{L_i} \vec{E}\cdot d\vec{s}, \quad \hat{\tilde{b}}_i = \int_{A_i} \vec{B}\cdot d\vec{A}, \\ \hat{\tilde{d}}_i &= \int_{\tilde{A}_i} \vec{D}\cdot d\vec{A}, \quad \hat{h}_i = \int_{\tilde{L}_i} \vec{H}\cdot d\vec{s}, \quad \hat{\tilde{j}}_i = \int_{\tilde{A}_i} \vec{J}\cdot d\vec{A}. \end{aligned} \tag{1}$$

Using this kind of state variables, an exact representation of the integral form of Faraday's and Ampere's law applied to facets of the grids can be found. In matrix-vector form, the so-called *Maxwell's Grid Equations* [5] read

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$$\mathbf{C}\hat{\mathbf{e}} = -\frac{d}{dt}\hat{\tilde{\mathbf{b}}}, \qquad \mathbf{C}^T\hat{\mathbf{h}} = \frac{d}{dt}\hat{\tilde{\mathbf{d}}} + \hat{\tilde{\mathbf{j}}}, \tag{2}$$

with the *curl-matrix* $\mathbf{C}$ and the vectors of voltages and fluxes $\hat{\mathbf{e}}, \hat{\mathbf{h}}$ and $\hat{\tilde{\mathbf{d}}}, \hat{\tilde{\mathbf{b}}}, \hat{\tilde{\mathbf{j}}}$, respectively. The approximations of the method finally take place in the material matrices (the discrete constitutive relations), given here for the linear case:

$$\hat{\tilde{\mathbf{d}}} = \mathbf{M}_\varepsilon \hat{\mathbf{e}}, \quad \hat{\tilde{\mathbf{b}}} = \mathbf{M}_\mu \hat{\mathbf{h}}, \quad \hat{\tilde{\mathbf{j}}} = \mathbf{M}_\kappa \hat{\mathbf{e}} + \hat{\tilde{\mathbf{j}}}_S \tag{3}$$

($\hat{\tilde{\mathbf{j}}}_S$ = source currents). For *dual orthogonal* grid systems $\mathbf{M}_\varepsilon$, $\mathbf{M}_\mu$, and $\mathbf{M}_\kappa$ are diagonal matrices.

If we apply FIT on Cartesian grids (the 'Yee-cell') and use the leap-frog scheme for the time-integration of (2), we obtain the same update equations as in FDTD. Thus, (2) can be considered to describe also the spatial discretization of FDTD [6].

In frequency domain we can eliminate the magnetic voltages $\hat{\mathbf{h}}$ in (2) and obtain the discrete curl-curl-equation (for the lossless case with $\mathbf{M}_\kappa = \mathbf{0}$):

$$\underbrace{(\mathbf{M}_\varepsilon^{-1}\mathbf{C}^T\mathbf{M}_\mu^{-1}\mathbf{C}}_{\mathbf{A}_{CC}} - \omega^2\mathbf{I})\hat{\mathbf{e}} = -j\omega\mathbf{M}_\varepsilon^{-1}\hat{\tilde{\mathbf{j}}}_S . \tag{4}$$

It can be easily shown that the curl-curl system matrix $\mathbf{A}_{CC}$ has only real eigenfrequencies ω_i, corresponding to undamped oscillating resonant modes in lossless structures. It is a standard task of many electromagnetic simulation codes to calculate the dominant eigensolutions of $\mathbf{A}_{CC}$, i.e. the resonant modes with lowest frequencies $\omega_i > 0$. These modes will be used in this paper to determine the averaged material quantities in a frequency range around the resonance, thus avoiding a costly time domain simulation with long transients until steady state.

For the simulation of metamaterials in time domain, we would need an incident wave excitation as well as implementations of open and periodic boundary conditions. Such open boundary conditions, if transformed back to frequency domain, would introduce losses in our model, leading to a complex system matrix and many difficulties in solving the corresponding eigenvalue equation. However, we will demonstrate, that at least for a non-oblique incidence of plane waves it is sufficient to consider only one element of the lattice and the lossless formulation given by (4).

B. Extraction of Effective Material Parameters

Once we have calculated a monofrequent field pattern (a solution $\hat{\mathbf{e}}$ of (4) for a given frequency and the related vectors $\hat{\tilde{\mathbf{d}}}, \hat{\tilde{\mathbf{b}}}, \hat{\mathbf{h}}$), the next step is to extract averaged field quantities. This averaging process, motivated by a macroscopic view of the cells of the lattice [1], is performed according to (e.g. for the magnetic x-components)

$$H_{x,av}(\omega) = \frac{1}{L_x}\int_{L_x} \vec{H}(\omega,\vec{r})\cdot d\vec{r},$$
$$B_{x,av}(\omega) = \frac{1}{S_x}\int_{S_x} \vec{B}(\omega,\vec{r})\cdot d\vec{A}, \tag{5}$$

where L_x and S_x are the corresponding edge and the surface of the cell, respectively. The related effective material coefficient is finally defined by

$$B_{x,av}(\omega) = \mu_0\,\mu_{eff,x}(\omega)\; H_{x,av}(\omega) . \tag{6}$$

For the discrete solutions $\hat{\mathbf{h}}(\omega)$ and $\hat{\tilde{\mathbf{b}}}(\omega) = \mathbf{M}_\mu\hat{\mathbf{h}}(\omega)$ the integrations in (5) can be represented by simple summations of specific voltage or flux components (cf. their definition in (1)):

$$H_{x,av}(\omega) = \mathbf{p}_{Lx}^T\hat{\mathbf{h}}(\omega), \qquad B_{x,av}(\omega) = \mathbf{p}_{Sx}^T\mathbf{M}_\mu\hat{\mathbf{h}}(\omega) . \tag{7}$$

Here the integration paths as well as the averaging coefficients are included in the *path vectors* $\mathbf{p}_{Lx}$ (containing only $\{0,\pm 1/L_x\}$) and $\mathbf{p}_{Sx}$ (containing only $\{0,\pm 1/S_x\}$).

III. Modal Approach

A. Basic Approach

In the modal approach [4], the solution of the curl-curl equation (4) is expressed as a sum of (ortho-normalized) eigenvectors of the system matrix:

$$\hat{\mathbf{e}}(\omega) = \sum \alpha_i \hat{\mathbf{e}}_i \tag{8}$$

with

$$\mathbf{A}_{CC}\hat{\mathbf{e}}_i = \omega_i^2\hat{\mathbf{e}}_i \;\text{ and }\; \hat{\mathbf{e}}_i^T\mathbf{M}_\varepsilon\hat{\mathbf{e}}_j = \delta_{ij} . \tag{9}$$

From (4) we obtain the simple formula for the unknown coefficients α_i:

$$\alpha_i(\omega) = \frac{-j\omega\;\hat{\mathbf{e}}_i^T\hat{\tilde{\mathbf{j}}}_S}{\omega_i^2 - \omega^2} . \tag{10}$$

Thus, instead of solving a linear system of equations for each frequency point, we can also determine the eigensolutions of the curl-curl system matrix and evaluate the explicit formulas (10) and (8).

Of course, for an exact solution of (4) using this approach all eigensolutions of the system matrix would be

needed. For realistic problem sizes this can not be achieved, and we have to use the incomplete expansion

$$\hat{\mathbf{e}}(\omega) = \sum_{1}^{p} \alpha_i(\omega)\hat{\mathbf{e}}_i + \hat{\mathbf{e}}_{corr}(\omega) \qquad (11)$$

with $p \ll \dim(\mathbf{A}_{CC})$ (typically p ≤ 10..100) and a correction term $\hat{\mathbf{e}}_{corr}(\omega)$.

From the result for the coefficients $\alpha_i(\omega)$ in (10) it is obvious, that the dominant modes (having the strongest frequency dependency) are as expected those with resonance frequencies $\omega_i \approx \omega$, and as a minimum a certain number of these modes must be considered in the expansion. Moreover, the contribution of the remaining (non-considered) modes can be assumed to be approximately constant in the near of the resonance. This leads to a simple correction approach, where a *constant* $\hat{\mathbf{e}}_{corr}$ is calculated as a solution of (4) at a fixed frequency within the range of interest. Since a good start vector for an iterative solvers is available with the modal part of (11), this solution of a system of equations is computationally cheap.

A more sophisticated correction approach, involving the solution of a second eigenvalue problem with varied boundary conditions, has been proposed in [4].

B. Excitation Strategy

The extraction of effective material parameters requires a monofrequent field solution in the lattice, or at least in one cell of the lattice (from a simulation including periodic boundaries.)

The simplest case of an appropriate setup is shown in Fig. 1: The periodicity in the transversal directions is realized by two pairs of magnetic (PMC) and electric (PEC) boundary conditions, respectively. Thus, the field pattern of the exciting planar wave is equivalent to a *waveguide excitation* (parallel plate guide) of the structure.

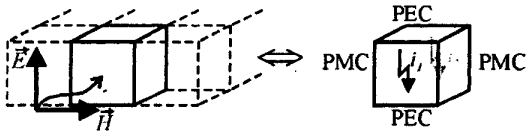

Fig. 1. Modeling of the periodic lattice by a single cell with appropriate boundary conditions and excitations.

This setup allows to model the cell as a two-port-device with generalized input currents i_1 and i_2, and output voltages u_1, and u_2, respectively. To obtain a periodic solution in the direction of the incident wave, these port quantities must satisfy

$$u_2 = u_1 \cdot e^{-i\varphi}, \quad i_2 = -i_1 \cdot e^{-i\varphi}, \qquad (12)$$

with $\varphi = k \cdot l_z$ the phase angle of the wave and l_z the length of one cell. Using

$$\begin{pmatrix} u_1 \\ u_1 \cdot e^{-i\varphi} \end{pmatrix} = \begin{pmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{pmatrix} \begin{pmatrix} i_1 \\ -i_1 \cdot e^{-i\varphi} \end{pmatrix}, \qquad (13)$$

where the system's impedance matrix **Z** can readily be calculated by the modal approach above, this leads to the *dispersion relation* between k and ω of the macroscopic wave:

$$e^{-ik/l_x} = \gamma \pm \sqrt{\gamma^2 - 1}, \quad \gamma = \frac{Z_{11}(\omega) + Z_{22}(\omega)}{2 \cdot Z_{12}(\omega)} \qquad (14)$$

Note that here also complex wave numbers k (describing attenuated waves) are allowed, and the sign in (14) has to be chosen accordingly.

The exciting current distribution at the port planes is calculated from the magnetic field pattern of the 2D waveguide mode (solution of a related discrete eigenvalue problem for its cross-section).

C. Metamaterial Simulation

Now we have all components to perform the simulation of the metamaterials:

1) Determine the discrete mode pattern at the port planes of one cell of the array, and transform them into equivalent surface currents.
2) Calculate a number of 3D eigenmodes of the cell with PMC boundaries of at the ports.
3) Calculate the correction vector(s).
4) For each frequency:
   a) Calculate the impedance matrix from the modal approach using (10) and (11).
   b) Calculate the phase angle according to (14) and construct the input currents at both ports.
   c) Calculate field solutions for this excitation.
   d) Extract averaged fields and calculate material parameters ε_{eff} and μ_{eff}.

The main computational cost in this procedure is due to the solution of the 3D eigenvalue problem (step 2). Once the coupling coefficients $\hat{\mathbf{e}}_i^T \bar{\bar{\mathbf{j}}}_S$ between these modes and the excitation currents are available, the remaining steps require neglectible computation time for an arbitrary number of frequency points. By a proper implementation of the formulas it can even be achieved that the field solutions (step 4c) need not be explicitly constructed and stored.

II. Numerical Results

Fig. 2 (taken from [3]) shows a metamaterial consisting of an array of split ring resonators (SRRs) and accompanying wires, which has been subject to measurements as well as simulations before ([3], and in a simplified form in [2]). In the grid model – all simulations are based on the commercial code CST Microwave Studio (MWS, [7]) – one cell of the lattice is discretized with a rather coarse mesh with only 1,980 grid points (also shown in Fig. 2). Due to the small dimensions of the SRR, this is still equivalent to more than 100 lines per wavelength. To be able to model the geometric details of the SRR in this mesh we apply the PBA™-technique incorporated in MWS.

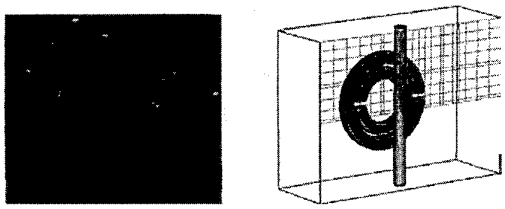

Fig. 2. SRR-type metamaterial (taken from [3]) and one cell of the array in the simulation model.

As a reference we performed an eigenmode analysis (with the same grid model) with periodic boundaries, as described in [2]. Here a complex hermitian eigenmode problem has to be solved several times for a varying phase angle φ between 0 to 180°. From the eigenfrequencies one gets the dispersion relation $\omega(k)$, and the eigenvectors can be used for the material averaging.

In the modal approach (with and without correction term) between 1 and 12 eigenmodes are used. Like in [2], models with and without the wire have been studied.

The resulting curve for the effective permeability (cf. Fig. 3) shows the desired resonance at approximately 3.66 GHz. It turns out, that with the correction term one single mode is sufficient to reproduce the frequency behavior of μ_{eff}, whereas without correction at least 10 modes are needed for an accurate result. The agreement with the reference is very good.

II. Conclusions

For the computation of effective material parameters in metamaterials a modal approach in combination with the Finite Integration Technique (or FDTD) has been presented. The field solution in single cells of the array is constructed by an incomplete expansion in eigenmodes of the closed structure. For the highly resonant behavior of metamaterials the new method turns out to be superior to time domain methods, since only a small number of modes is needed to reproduce the typical resonance curves. It has also been demonstrated that a correction term compensating the missing modes is very important to obtain accurate results with moderate cost.

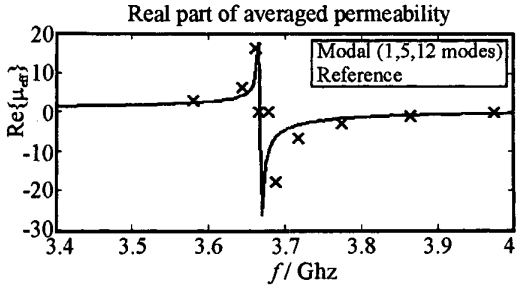

Fig. 3. Simulation results: Real part of the effective permeability $Re\{\mu_{eff}\}$: Reference solution (periodic eigenvalue analysis), modal approach with correction and varying number of considered eigenmodes (indistinguishable curves).

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