Stable and efficient ABCs for graded mesh FDTD simulations

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Abstract—**Well known Absorbing Boundary Conditions show instabilities if used for graded mesh FDTD simulations of structures on high permittivity substrates. This paper proposes a PML like absorber which is unconditionally stable. Reflection factors of less than -70 dB have been achieved for coplanar waveguide termination.**

I. Introduction

Perfectly Matched Layer (PML) boundary conditions [1], [2] have been found instable in conjunction with layered media [3]. On graded mesh FDTD analysis of coplanar strip line resonators coupled magnetically to a feeding coplanar waveguide on a $\varepsilon_r = 27$ substrate, we found that retarded boundary conditions as well as first order Mur ABCs [4] yield instabilities, too. Since long (and accurate) time series of voltages and currents are needed to analyze resonant structures like this, the simulation results were completely unusable.

As a solution, this paper proposes a PML like absorber we call matched layer (ML) which consists of material with electric and magnetic losses. In contrast to the PML concept the field components are not split and the material is isotropic.

II. Stability analysis for a lossy graded mesh FDTD method

A FDTD scheme for treatment of graded meshes for inhomogeneous material with electric and magnetic losses in a short operator formulation is the basis for the absorber presented here. An improved version of the equivalent circuit formulation in [5] is then used to prove the stability of the method and to derive a stability criterion.

Figure 1 shows the unit cell of the well known Yee FDTD scheme [6]. Field components as well as the cell sizes and the material properties are functions of the discrete position $X = (i, j, k)^{\mathrm{T}}$. Field components and other properties accounted to the cell X are shown in the figure. For simpler writing, component and direction indices are numbered in a modulo three sense, e. g. $E_0 \equiv E_{\mathrm{x}}$, $E_1 \equiv E_{\mathrm{y}}$, $E_2 \equiv E_{\mathrm{z}}$ and again $E_3 \equiv E_{\mathrm{x}}$ and $E_{-1} \equiv E_{\mathrm{z}}$. Upper indices E rsp. H are used for the electric rsp. magnetic conductivity σ^{E} rsp. σ^{H} and for the sub cell sizes Δ^{E} and Δ^{H}. A lower index "+" means $\nu + 1$, a "-" stands for $\nu - 1$. The shift operators ξ_ν and $\widehat{\xi}_\nu$ are defined by $\xi_\nu H_\mu(X) = H_\mu(X + \mathcal{E}_\nu)$ and $\widehat{\xi}_\nu H_\mu(X) = H_\mu(X - \mathcal{E}_\nu)$, with the unit vector in ν direction $\mathcal{E}_\nu$.

The time continuous Yee scheme for lossy material and graded mesh discretization is

$$
\begin{aligned}
(\varepsilon_\nu \partial_t + \sigma_\nu^{\mathrm{E}}) E_\nu &= \frac{1}{\Delta_+^{\mathrm{H}}}(\xi_+ - 1) H_- - \frac{1}{\Delta_-^{\mathrm{H}}}(\xi_- - 1) H_+, \\
(\mu_\nu \partial_t + \sigma_\nu^{\mathrm{H}}) H_\nu &= \frac{1}{\Delta_+^{\mathrm{E}}}(\widehat{\xi}_+ - 1) E_- - \frac{1}{\Delta_-^{\mathrm{E}}}(\widehat{\xi}_- - 1) E_+
\end{aligned}
\tag{1}
$$

with

$$
\begin{aligned}
\varepsilon_\nu &= \frac{1}{4}\left(1 + \widehat{\xi}_+ + \widehat{\xi}_- + \widehat{\xi}_- \widehat{\xi}_+\right) \varepsilon, \\
\sigma_\nu^{\mathrm{E}} &= \frac{1}{4}\left(1 + \widehat{\xi}_+ + \widehat{\xi}_- + \widehat{\xi}_- \widehat{\xi}_+\right) \sigma^{\mathrm{E}}, \\
\mu_\nu &= \frac{1}{4}(1 + \xi_+ + \xi_- + \xi_- \xi_+) \mu, \\
\sigma_\nu^{\mathrm{H}} &= \frac{1}{4}(1 + \xi_+ + \xi_- + \xi_- \xi_+) \sigma^{\mathrm{H}}.
\end{aligned}
\tag{2}
$$

For stability analysis, an equivalent circuit formulation for (1) is proposed in [5]. The graded mesh FDTD scheme used here, requires magnetic and electric voltages to be introduced to maintain symmetry of the equivalent circuit. With $\theta^{\mathrm{E}}_{\nu} = E_\nu \Delta^{\mathrm{E}}_{\nu}$ and $\theta^{\mathrm{H}}_{\nu} = H_\nu \Delta^{\mathrm{H}}_{\nu}$ equation (1) yields[1]

$$\begin{aligned}(C_\nu \partial_t + G_\nu)\theta^{\mathrm{E}}_{\nu} &= (\xi_+ - 1)\theta^{\mathrm{H}}_{-} - (\xi_- - 1)\theta^{\mathrm{H}}_{+},\\ (L_\nu \partial_t + R_\nu)\theta^{\mathrm{H}}_{\nu} &= (\widehat{\xi}_+ - 1)\theta^{\mathrm{E}}_{-} - (\widehat{\xi}_- - 1)\theta^{\mathrm{E}}_{+},\end{aligned} \tag{3}$$

with

$$\begin{aligned}C_\nu &= \frac{\Delta^{\mathrm{H}}_{+}\Delta^{\mathrm{H}}_{-}}{\Delta^{\mathrm{E}}_{\nu}}\varepsilon_\nu, & G_\nu &= \frac{\Delta^{\mathrm{H}}_{+}\Delta^{\mathrm{H}}_{-}}{\Delta^{\mathrm{E}}_{\nu}}\sigma^{\mathrm{E}}_{\nu},\\ L_\nu &= \frac{\Delta^{\mathrm{E}}_{+}\Delta^{\mathrm{E}}_{-}}{\Delta^{\mathrm{H}}_{\nu}}\mu_\nu, & R_\nu &= \frac{\Delta^{\mathrm{E}}_{+}\Delta^{\mathrm{E}}_{-}}{\Delta^{\mathrm{H}}_{\nu}}\sigma^{\mathrm{H}}_{\nu}.\end{aligned} \tag{4}$$

The equivalent circuit then has the same structure as in [5].

To prove the stability of the *infinite* time continuous scheme,

$$\begin{aligned}&\sum_{X,\nu}\frac{1}{2}\partial_t[C_\nu(\theta^{\mathrm{E}}_{\nu})^2 + L_\nu(\theta^{\mathrm{H}}_{\nu})^2] + G_\nu(\theta^{\mathrm{E}}_{\nu})^2 + R_\nu(\theta^{\mathrm{H}}_{\nu})^2\\ =&\sum_{X,\nu}\theta^{\mathrm{E}}_{\nu}(C_\nu\partial_t + G_\nu)\theta^{\mathrm{E}}_{\nu} + \theta^{\mathrm{H}}_{\nu}(L_\nu\partial_t + R_\nu)\theta^{\mathrm{H}}_{\nu}\\ =&\sum_{X,\nu}\theta^{\mathrm{E}}_{\nu}[(\xi_+ - 1)\theta^{\mathrm{H}}_{-} - (\xi_- - 1)\theta^{\mathrm{H}}_{+}]\\ +&\sum_{X,\nu}\theta^{\mathrm{H}}_{\nu}[(\widehat{\xi}_+ - 1)\theta^{\mathrm{E}}_{-} - (\widehat{\xi}_- - 1)\theta^{\mathrm{E}}_{+}]\\ =&\sum_{X,\nu}\theta^{\mathrm{E}}_{\nu}\xi_+\theta^{\mathrm{H}}_{-} - \theta^{\mathrm{E}}_{\nu}\theta^{\mathrm{H}}_{-} - \theta^{\mathrm{E}}_{\nu}\xi_-\theta^{\mathrm{H}}_{+} + \theta^{\mathrm{E}}_{\nu}\theta^{\mathrm{H}}_{+}\\ +&\sum_{X,\nu}\eta_+\xi_+\theta^{\mathrm{H}}_{\nu}\widehat{\xi}_+\theta^{\mathrm{E}}_{-} - \eta_+\theta^{\mathrm{H}}_{\nu}\theta^{\mathrm{E}}_{-} - \eta_-\xi_-\theta^{\mathrm{H}}_{\nu}\widehat{\xi}_-\theta^{\mathrm{E}}_{+} + \eta_-\theta^{\mathrm{H}}_{\nu}\theta^{\mathrm{E}}_{+}\\ =&0\end{aligned} \tag{5}$$

is used, where the prefix operators of all terms in the last sum do the necessary substitutions to get the zero result. Component substitutions are done by the η operator[2], e.g.

$$\begin{aligned}\eta_+ H_\mu &= H_{\mu+1},\\ \eta_- H_\mu &= H_{\mu-1},\\ \eta_+\xi_+\theta^{\mathrm{H}}_{\nu}\widehat{\xi}_+\theta^{\mathrm{E}}_{-} &= \eta_+\theta^{\mathrm{E}}_{-}\xi_+\theta^{\mathrm{H}}_{\nu} = \theta^{\mathrm{E}}_{\nu}\xi_-\theta^{\mathrm{H}}_{+}.\end{aligned} \tag{6}$$

Equation (5) yields

$$\frac{1}{2}\partial_t\sum_{X,\nu}C_\nu(\theta^{\mathrm{E}}_{\nu})^2 + L_\nu(\theta^{\mathrm{H}}_{\nu})^2 = -\sum_{X,\nu}G_\nu(\theta^{\mathrm{E}}_{\nu})^2 + R_\nu(\theta^{\mathrm{H}}_{\nu})^2 \leq 0, \tag{7}$$

and since $C_\nu, L_\nu > 0$ and $G_\nu, R_\nu \geq 0$ the stability of the time continuous scheme is proved.

For stability analysis of the time discrete scheme, the lossless Yee scheme is considered, since this is the worst case. The equivalent discrete wave equation derived from (1) is

$$\begin{aligned}\partial_t^2\theta^{\mathrm{E}}_{\nu} = \frac{1}{C_\nu}[&+(\xi_+ - 1)\frac{1}{L_-}(\widehat{\xi}_\nu - 1)\,\eta_+\\ &-(\xi_+ - 1)\frac{1}{L_-}(\widehat{\xi}_+ - 1)\\ &-(\xi_- - 1)\frac{1}{L_+}(\widehat{\xi}_- - 1)\\ &+(\xi_- - 1)\frac{1}{L_+}(\widehat{\xi}_\nu - 1)\,\eta_-]\,\theta^{\mathrm{E}}_{\nu}\\ =&O_\Delta\,\theta^{\mathrm{E}}_{\nu}\end{aligned} \tag{8}$$

and the usual time discretization yields

$$O_{\mathrm{tt}}\,\theta^{\mathrm{E}} = \frac{(\xi_{\mathrm{t}} - 1)(1 - \widehat{\xi}_{\mathrm{t}})}{\Delta_{\mathrm{t}}^2}\,\theta^{\mathrm{E}} = O_\Delta\,\theta^{\mathrm{E}}, \tag{9}$$

with the time step Δ_{t} and the time shift operators ξ_{t} and $\widehat{\xi}_{\mathrm{t}}$.

The adjoined operator of O_Δ (corresponding to the transposition of the equivalent matrix) is

$$\begin{aligned}O_\Delta{}^{\mathrm{a}} = &+\eta_-(\xi_\nu - 1)\frac{1}{L_-}(\widehat{\xi}_+ - 1) - (\xi_+ - 1)\frac{1}{L_-}(\widehat{\xi}_+ - 1)\\ &- (\xi_- - 1)\frac{1}{L_+}(\widehat{\xi}_- - 1) + \eta_+(\xi_\nu - 1)\frac{1}{L_+}(\widehat{\xi}_- - 1),\end{aligned} \tag{10}$$

[1] If the Yee scheme is implemented like this on a computer, one multiplication per time step and field component can be saved.

[2] It is worth noting, that

- the $\xi_+ = \xi_{\nu+1}$ operator refers to a fixed direction $\nu + 1$, the η_+ operator does not and
- the ξ and η operators do not commute, e.g. $\eta_+\xi_+ = \xi_-\eta_+$ or $\eta_+\xi_- = \xi_\nu\eta_+$.

because e.g. $\eta_-^a = \eta_+$, $\widehat{\xi}^a = \xi$ and because the adjoined operator has to be written as reverse order product. It can be seen, that the operator is self adjoined.

Thus it is known, that

1. stability analysis can be restricted to the eigenfunctions of O because all possible θ^E can be written as linear combinations of eigenfunctions of the self adjoined operator.
2. all eigenvalues of the self adjoined operator O_Δ are real.
3. all eigenvalues of O_Δ are negative or zero, because else (8) would have instable solutions and stability is proved above.

An estimate for the spectral radius of O_Δ is

$$r(O_\Delta) \leq 16 \left(\frac{1}{L_V C_V} \right)_{\max}, \tag{11}$$

because the norm of η and ξ is one and (8) yields, that O_Δ can be written as a sum of 16 terms. The difference equation now is

$$O_{tt}\, \theta^E \quad = \quad -\lambda^2\, \theta^E. \tag{12}$$

Solutions are $\theta^E(T) = e^{aT}$, where T is the discrete time. Stability is reached, if no solutions with a positive real part of a exist, this means $\lambda^2 \Delta_t^2 < 4$. Thus, a stability criterion for the graded mesh FDTD is

$$\left(\frac{1}{L_V C_V} \right)_{\max} \Delta_t^2 < \frac{1}{4}. \tag{13}$$

III. The ML absorber for the graded mesh FDTD method

The Matched Layer is introduced by the same matching condition used in the PML concept, e.g. the electric time constant τ_E and the magnetic time constant τ_H must be equal,

$$\tau = \tau_E = \varepsilon/\sigma^E \quad = \quad \tau_H = \mu/\sigma^H. \tag{14}$$

to match the wave impedance outside the absorber. This concept is known to perfectly absorb plane waves with normal[3] incidence on a homogeneous absorber.

Normal incidence of a plane wave yields

$$\begin{aligned} \gamma &= \sqrt{(j\omega\varepsilon + \sigma^E)(j\omega\mu + \sigma^H)} \\ &= j\sqrt{\mu\varepsilon}(1 \pm j\frac{1}{\tau}) \\ &= \alpha + j\beta, \\ \alpha &= \sqrt{\mu\varepsilon}\frac{1}{\tau}, \end{aligned} \tag{15}$$

where α is the absorption coefficient.

The reflection coefficient of an absorber with a thickness d and smoothly increasing losses $1/\tau(x)$ terminated by an electric or magnetic boundary condition then is

$$S_{11} = e^{-2\,\sqrt{\mu\varepsilon} \int_0^d \frac{1}{\tau}(x)\, dx}. \tag{16}$$

IV. Application to coplanar transmission line termination

In this paper, ML absorbers have been successfully used for stable coplanar transmission line termination on a $\varepsilon_r = 27$ substrate. In the substrate as well as in the air–filled regions, (14) is used to calculate the losses.

The losses increase smoothly with a $1/\tau = A(x/d)^n$ dependence, were $1/A$ is the minimum time constant and d the absorber's thickness. The electric conductivity σ^E is sampled at the center point of the electric sub cell of the Yee scheme, the magnetic conductivity σ^H at the center point of the magnetic sub cell.

As absorber parameters, its thickness m (in Cells), the exponent n and the absorption of its continuous and homogeneous counterpart

$$S_{11}^{co} \quad = \quad e^{-\frac{2Ad}{v_{ph}(n+1)}} \tag{17}$$

were used.

[3]PML's field component splitting and anisotropy is mainly introduced to handle arbitrary angles of incidence.

Figure 2 shows the reflection coefficient of ML absorbers terminating coplanar waveguides. The parameters were S_{11}^{co} = -80 dB, n = 1.25 and m = 6 rsp. 8 cells. For the test, the structure is discretized homogeneously (Δ = 10 μm) in propagation direction. The other directions are discretized unevenly ($\Delta \in [2.5\mu\text{m}, 10\mu\text{m}]$). The absorbers yield good performance at frequencies up to 400 GHz with reflections less than -55 dB.

V. Conclusions

Stability problems were observed in graded mesh FDTD simulations with traditional ABCs making it impossible to analyze resonant structures. A Matched Layer concept is proposed in this paper, proved to be stable and used for coplanar waveguide termination with excellent results.

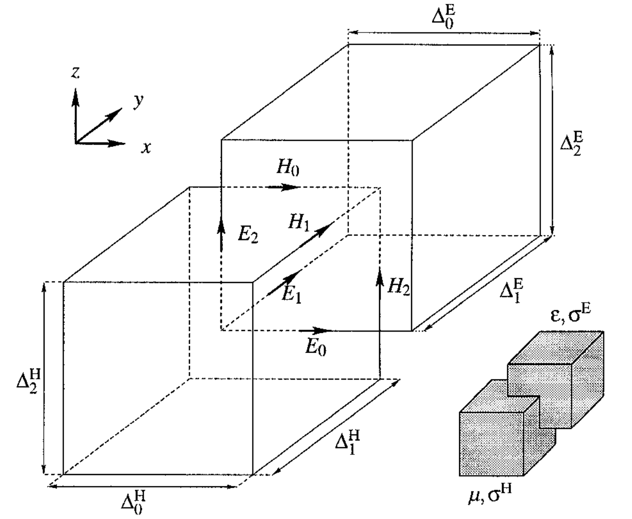

Fig. 1. Yee cell at the position X with the field components and parameters accounted to this cell.

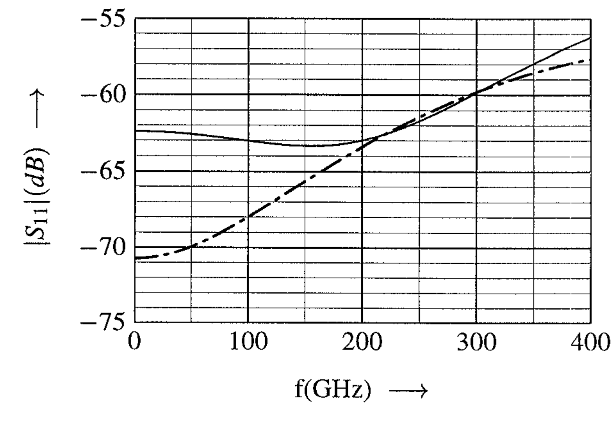

Fig. 2. Reflection coefficient $|S_{11}|$ of ML absorbers terminating w = 15 μm and s = 5 μm coplanar waveguides. The solid line is for a 6 cell absorber, the other line for a 8 cell one.

References

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