Modelling Dispersive Media Using the Finite Integration Technique

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Abstract

Since simulation of broadband applications have gained in importance in the last years, the dispersive characteristics of various materials must not be neglected anymore. As a result many frequency dependent FDTD methods have been set up which in most cases model special dispersions of low order. On foundation of discrete system analysis we present an algorithm applicable to arbitrary material dispersions up to 2^{nd} order derived from a general approach [1]. The applicability of the presented method is demonstrated with an example using a rectangular waveguide filled with dielectric layers with different dispersion characteristics.

Introduction

The formulation of the *Finite Integration Technique* (FIT) according to Weiland [2] provides a general spatial discretization scheme usable for different electromagnetic applications of arbitrary geometry, e.g. static problems or calculations in frequency and time domain. In our paper we refer to the *Maxwell's Grid Equations* (MGE) (1)-(4) and material relations (5)-(7) given by

$$\mathbf{C}\,\mathbf{D}_s\,\mathbf{e} = -\mathbf{D}_A\,\dot{\mathbf{b}} \qquad (1)$$
$$\tilde{\mathbf{C}}\,\tilde{\mathbf{D}}_s\,\mathbf{h} = \tilde{\mathbf{D}}_A\,\dot{\mathbf{d}} \qquad (2)$$
$$\tilde{\mathbf{S}}\,\tilde{\mathbf{D}}_A\,\mathbf{d} = \mathbf{q} \qquad (3)$$
$$\mathbf{S}\,\mathbf{D}_A\,\mathbf{b} = \mathbf{0} \qquad (4)$$

$$\mathbf{d} = \mathbf{D}_\epsilon\,\mathbf{e} \qquad (5)$$
$$\mathbf{b} = \mathbf{D}_\mu\,\mathbf{h} \qquad (6)$$
$$\mathbf{j} = \mathbf{D}_\kappa\,\mathbf{e}. \qquad (7)$$

The geometry is discretized on a dual orthogonal grid system with $\mathbf{e}$, $\mathbf{b}$ located on the normal grid G and $\mathbf{d}$, $\mathbf{h}$ on the dual grid $\tilde{G}$. Correspondent to that the analytical curl operator results in the curl matrices $(\mathbf{C}, \tilde{\mathbf{C}})$ and the divergence operator in the source matrices $(\mathbf{S}, \tilde{\mathbf{S}})$. In the same way the grid resolution is contained in $(\mathbf{D}_s, \tilde{\mathbf{D}}_s)$ representing the grid lines and $(\mathbf{D}_A, \tilde{\mathbf{D}}_A)$ the belonging areas. If the material is assumed to be frequency independent and isotropic, we have diagonal matrices $\mathbf{D}_\epsilon$ and $\mathbf{D}_\mu$ describing the material relations. It can be shown, that the mentioned spatial discretization does not produce any instability since the discrete Maxwell equations fulfil energy and charge conservation [2].

Applying the well-known leap-frog scheme to the FIT formulas we can write (1,2) in form of two recursive update equations with $\mathbf{e}$ and $\mathbf{b}$ as the calculated field variables:

$$\mathbf{b}^{n+1} = \mathbf{b}^n - \Delta t\,\mathbf{D}_A^{-1}\,\mathbf{C}\,\mathbf{D}_s\,\mathbf{e}^{n+1/2} \qquad (8)$$
$$\mathbf{e}^{n+3/2} = \mathbf{e}^{n+1/2} + \Delta t\,\mathbf{D}_\epsilon^{-1}\,\tilde{\mathbf{D}}_A^{-1}\,\tilde{\mathbf{C}}\,\tilde{\mathbf{D}}_s\,\mathbf{D}_\mu^{-1}\,\mathbf{b}^{n+1}. \qquad (9)$$

Using a homogeneous equidistant grid these equations reduce to the standard finite-difference time-domain ($FDTD$) algorithm according to Yee [3]. Now stability due to time discretization is restricted to a certain interval, namely given by the Courant condition in free-space

$$\Delta t = \left(c_0 \sqrt{\left[\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right]} \right)^{-1} . \tag{10}$$

Since the sofar described time domain algorithm is restricted to non-dispersive materials many efforts have been made in the last years to expand it in a useful way. An important aspect in connection with these extensions is the guarantee of stability, because it is not possible to transfer the criterion (10) to frequency dependent materials in a straight forward manner. Apart from a quite practicable solution for this problem we have proposed in a recent paper [1] a very general time domain algorithm for dispersive materials. There we provide a stability analysis that is applicable to any frequency dependent time-domain method and therefore offers good possibilities for comparisons of the most important $(FD)^2TD$ algorithms [4, 5, 6, 7, 8, 9].

Algorithm for 2^{nd} Order Dispersion Models

Our approach is within the framework of system analysis by first considering a linear time-invariant system of n^{th} order, that can be described in general by a linear ordinary differential equation (ODE) of the same order. Rather then to discretize the n^{th} order ODE directly by replacing time derivatives by the corresponding central difference operator [8], we first apply the *state space formulation* to our system to derive an explicit algorithm for the time-domain simulation[1]. This formulation is chosen, since it employs matrices in its fundamental equations similar to the FIT-method and therefore both methods can easily be combined.
Since this procedure is presented in [1], we skip the derivation of the general approach and we present in the following the derived explicit update equation for a 2^{nd} order dispersion model. We choose a maximum order of two for the dispersion, since it covers the most significant dispersion models like Debye, Drude and Lorentz. Thus in the frequency domain the correspondent permittivity function reads as

$$\epsilon(\omega) = \underbrace{\beta_2}_{\epsilon_0\,\epsilon_\infty} + \frac{\beta_0 + j\omega \cdot \beta_1}{\alpha_0 + j\omega \cdot \alpha_1 - \omega^2 \cdot \alpha_2} . \tag{11}$$

The discretization in time is done by using exact integration of the first order ODE's. In general we derive from $dy(t)/dt = A\,y(t) + b(t)$ for the homogeneous case $y_h(t) = C\,exp(A\,t)$ and a special solution $y_s(t) = C(t)\,exp(A\,t)$ with $C(t) = -b/A\,exp(A\,t)$ by variation of parameters. The combination gives us the general solution and finally the expression for a discrete time step Δt

$$y^{n+1} = y^n\, e^{A\,\Delta t} + (e^{A\,\Delta t} - 1)/A\, b^{n+1/2}. \tag{12}$$

Here we like to mention that we assumed the function b as constant over the time step and separated by half a time step, where we choose the allocation of y at full time steps (alternatively one has to add $\Delta t/2$ to all signals in equation (12) in case that y is allocated at $t = (n+1/2)\,\Delta t$).

Unfortunately this is not the case in the ODE for the first state variable $\mathbf{z_1}$ (the polarization), since it includes the electric field on the right hand side, which is allocated at the same positions in time. In order to ensure a higher accuracy the electric field $\mathbf{e}^{n+1}$ is averaged by its existing neighbour values $\mathbf{e}^{n+1} = (\mathbf{e}^{n+3/2} + \mathbf{e}^{n+1/2})/2$ (see equation (16)). This finally leads to the following set of four coupled equations

$$
\begin{aligned}
\mathbf{b}^{n+1} &= \mathbf{b}^{n} - \Delta t\, \mathbf{D}_A^{-1}\, \mathbf{C}\, \mathbf{D}_s\, \mathbf{e}^{n+1/2} && (13)\\
\mathbf{z_2}^{n+1} &= \mathbf{D}_{exp_2}\, \mathbf{z_2}^{n} + (I - \mathbf{D}_{exp_2})\, \mathbf{D}_{\alpha_1}^{-1}\, (-\mathbf{D}_{\alpha_0}\, \mathbf{z_1}^{n+1/2} + \mathbf{D}_{b_2}\, \mathbf{e}^{n+1/2}) && (14)\\
\mathbf{e}^{n+3/2} &= \mathbf{D}_{exp_1}\, \mathbf{e}^{n+1/2} + (\mathbf{I} - \mathbf{D}_{exp_1})\, (-\mathbf{D}_{b_1}^{-1}\, \mathbf{z_2}^{n+1} + \mathbf{D}_{b_1}^{-1}\, \tilde{\mathbf{D}}_A^{-1} \tilde{\mathbf{C}}\, \tilde{\mathbf{D}}_s\, \mathbf{D}_{\mu}^{-1}\, \mathbf{b}^{n+1}) && (15)\\
\mathbf{z_1}^{n+3/2} &= \mathbf{z_1}^{n+1/2} + \Delta t\, \mathbf{z_2}^{n+1} + \Delta t\, \mathbf{D}_{b_1}\, \underbrace{\frac{1}{2}\, (\mathbf{e}^{n+3/2} + \mathbf{e}^{n+1/2})}_{\overline{\mathbf{e}}^{n+1}} && (16)
\end{aligned}
$$

with the matrices $\mathbf{D}_{b_1} = \mathbf{D}_{\beta_1} + \mathbf{D}_{\kappa}$; $\mathbf{D}_{b_2} = \mathbf{D}_{\beta_0} - \mathbf{D}_{\alpha_1}\, \mathbf{D}_{\beta_1}$; $\mathbf{D}_{exp_1} = exp(-\mathbf{D}_{\beta_2}^{-1}\, \mathbf{D}_{b_1}\, \Delta t)$ and $\mathbf{D}_{exp_2} = exp(-\mathbf{D}_{\alpha_1}\, \Delta t)$. In this algorithm we have also taken a static conductivity into account, that can easily be added by the extension of the matrix $\mathbf{D}_{b_1} = \mathbf{D}_{\beta_1} + \mathbf{D}_{\kappa}$, where the diagonal matrix $\mathbf{D}_{\kappa}$ represents the distribution of the conductivity inside the grid.

For simulating multiple media with different dispersion models up to second order in a single time domain calculation simultaneously, one has to set the dispersion model coefficients accordingly. In Table 1 they are summarized for the most relevant dispersion models, where the not listed coefficients are set to $\alpha_2 = 1$ and $\beta_2 = \epsilon_0\, \epsilon_\infty$ by definition.

Table 1: Permittivity model coefficients of Debye, Drude, Debye 2^{nd} order and Lorentz dispersion for the 2^{nd} order algorithm (13)-(16).

	Debye	Drude	Debye 2^{nd}	Lorentz
α_0	0	0	$1/(\tau_1\, \tau_2)$	ω_0^2
α_1	$1/\tau$	ν_c	$(\tau_1 + \tau_2)/(\tau_1\, \tau_2)$	δ
β_0	0	$\epsilon_0\, \Delta\epsilon\, \omega_p^2$	$\epsilon_0\, (\Delta\epsilon_1 + \Delta\epsilon_2)/(\tau_1\, \tau_2)$	$\epsilon_0\, \Delta\epsilon\, \omega_0^2$
β_1	$\epsilon_0\, \Delta\epsilon/\tau$	0	$\epsilon_0\, (\Delta\epsilon_1\, \tau_2 + \Delta\epsilon_2\, \tau_1)/(\tau_1\, \tau_2)$	0

Example

To verify the presented method, the 2^{nd} order algorithm is applied to an S-parameter calculation. In Figure 1 the test structure, a dielectric filled waveguide with different layers in propagation direction, is shown. Two frequency dependent materials with a 2^{nd} order dispersion are present (Debye 2^{nd} order, Lorentz medium; see Figure 2). The rest of the waveguide is filled with vacuum and throughout the waveguide the permeability equals $\mu = \mu_0$.

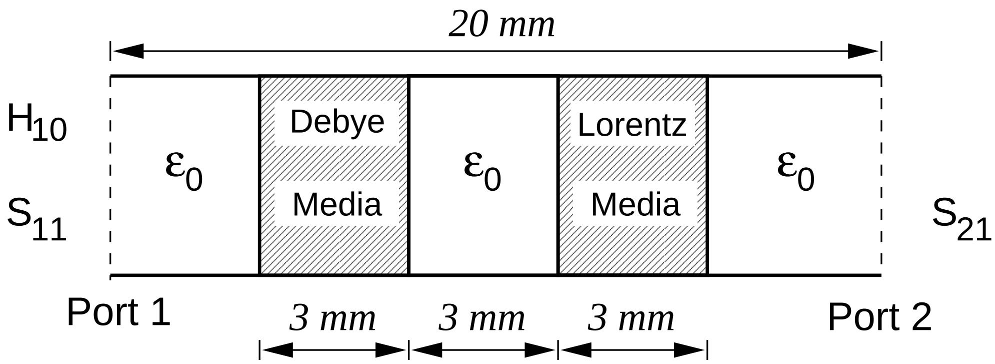

Figure 1: *Rectangular waveguide ($\mu = \mu_0$, port separation is 20 mm, cross-section 20 mm x 5 mm) with layers of different permittivities including ϵ_0 and dispersive permittivities Debye 2^{nd} order: $\epsilon_\infty = 1$; $\epsilon_{s_1} = \epsilon_{s_2} = 2$, $\tau_1 = 1/2/\pi/10e9\ s$, $\tau_2 = 1/2/\pi/20e9\ s$; Lorentz medium: $\epsilon_\infty = 1$; $\epsilon_{s_1} = 2$, $\delta = 20e9\ Hz$; $\omega_0 = 2\ \pi\ 20e9\ Hz$.*

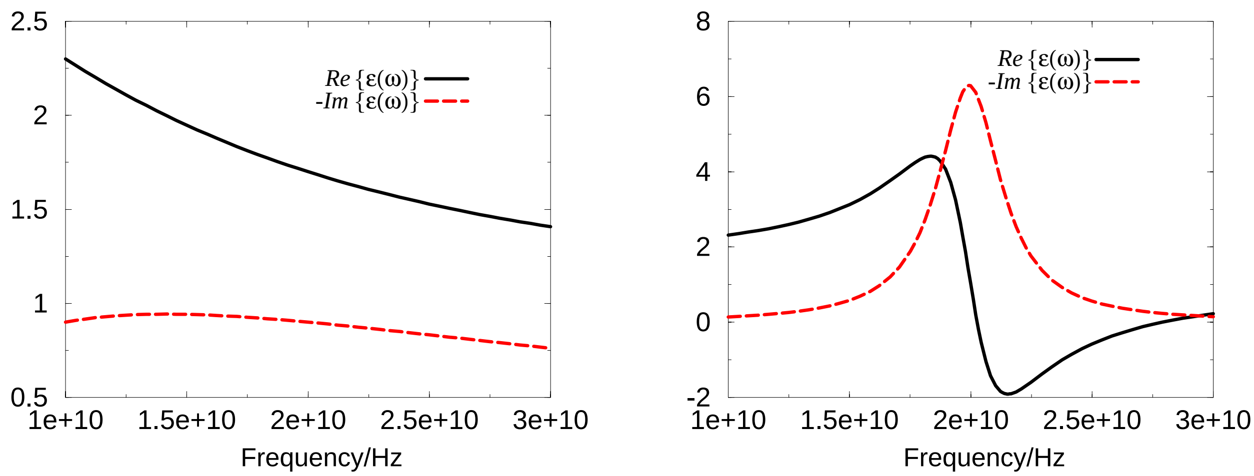

Figure 2: *a) Real and imaginary part of 2^{nd} order Debye material (frequency range $10\,GHz$-$30\,GHz$) b) Real and imaginary part of Lorentz material (frequency range $10\,GHz$-$30\,GHz$).*

We want to determine the amplitude and phase of the S_{11}, S_{21} parameters at the given ports separated by 20 mm for the frequency range 10 GHz - 30 GHz. Thus a broadband stimulation with the fundamental mode at port 1 in form of a Gaussian pulse modulated with a carrier frequency of 20 GHz results in the frequency domain in a Gaussian shaped excitation spectrum centred at 20 GHz with a 60dB bandwidth of 10 GHz. At the two ports a special waveguide boundary condition is used [11] that enables the simulation of an infinitely long waveguide ensuring a parasitic reflection of less than -120dB. To minimize grid dispersion the grid resolution is chosen such that it allows for thirty steps per wavelength for the highest frequency.
Thus the S-parameter calculation covers the following steps:

1. 2D-eigenvalue solver: calculation of the propagation modes inside the waveguide by discretizing the cross section of the waveguide ($\epsilon = \epsilon_0, \mu = \mu_0$).

2. 3D time domain simulation: broadband excitation with the fundamental mode at port 1

and monitoring the mode amplitude of the reflected wave at port 1 and the transmitted mode amplitude at port 2.

3. Post-processing: S-parameter calculation from the excitation and the monitored signals in the frequency domain by using the *Fast Fourier Transform* (FFT).

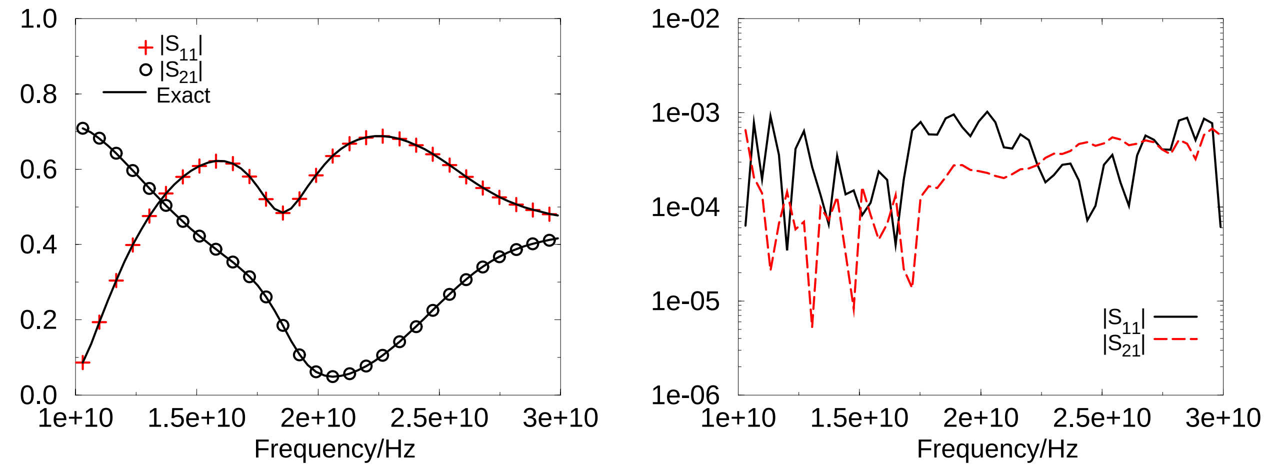

Figure 3: *Comparison of numerical results with analytical solution in the frequency range* $10\,GHz$-$30\,GHz$. *a) Absolute value of S-parameter* $S_{11},\ S_{21}$*; b) amplitude error of S-parameter* $|S_{11}|,\ |S_{21}|$.

Figure 3 presents the absolute value of S-parameter $S_{11},\ S_{21}$ compared with the analytical solution and the resulting amplitude error for the frequency range $10\,GHz$-$30\,GHz$. As it can be seen there is an excellent agreement of the numerical results with the exact solution. The absolute amplitude error is well below 10^{-3}.

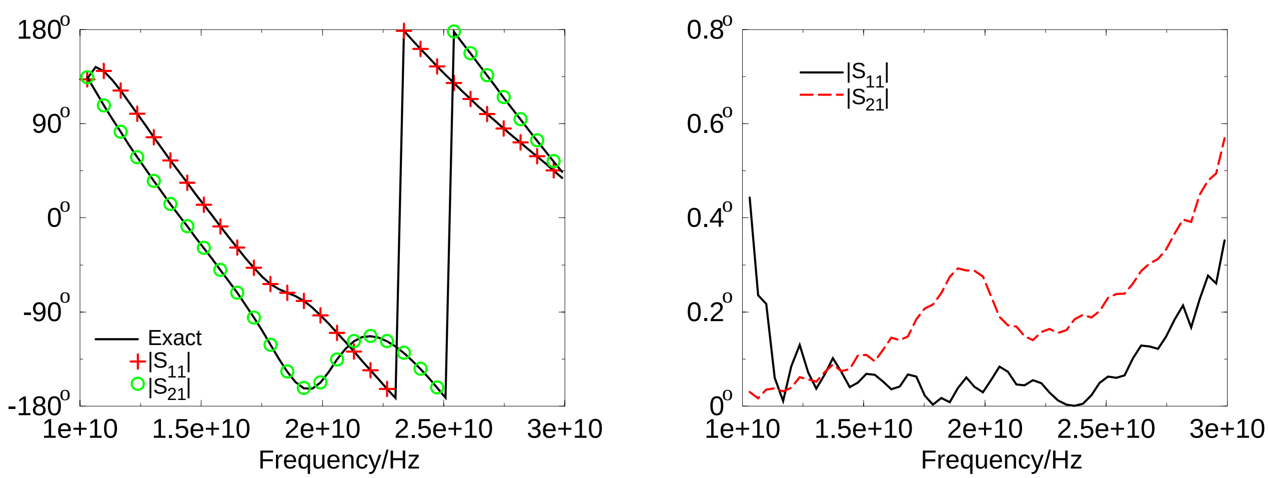

Figure 4: *Comparison of numerical results with analytical solution in the frequency range* $10\,GHz$-$30\,GHz$. *a) Phase of S-parameter* $S_{11},\ S_{21}$*; b) Phase error of S-parameter* $|S_{11}|,\ |S_{21}|$.

A similar good agreement in case of both S-parameter phase results shows Figure 4. Here the maximum absolute phase error is below 0.6^o.

Conclusion

In this paper we presented a very general possibility to extend the FIT algorithm for modelling dispersive media with a dispersion of 2^{nd} order. This algorithm was derived from a general approach based on system analysis with a state-space formulation. The additional state-variables correspond to physical properties, the polarisation und the polarisation current density. We demonstrated the good accuracy of our algorithm with an example of a rectangular waveguide filled with two layers of frequency dependent material of second order (Lorentz-Media and a 2^{nd} order Debye-Model).

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