

Dispersive Media in FDTD — Comparison of Recursive Convolution and Auxiliary Differential Equation Methods

T. O. Körner and W. Fichtner

Integrated Systems Laboratory, Swiss Federal Institute of Technology, 8092 Zürich, Switzerland

ABSTRACT

A new, efficient algorithm for modelling dispersive media in Finite Difference Time Domain (FDTD) methods is presented. It is based on the Auxiliary Differential Equation (ADE) formulation. Accuracy and efficiency are compared to other ADE implementations and to various Recursive Convolution (RC) methods.

INTRODUCTION

Various approaches for modelling frequency dependent material properties in finite-difference time-domain methods for electromagnetics have emerged in recent years. Appropriate treatment of material dispersion is important for simulating propagation of short pulses as well as for efficient modelling of propagation phenomena over a wide range of frequencies in optical as well as microwave regimes. The different methods are based on three main principles: The recursive computation of the convolution integral between electric field and time domain susceptibility [1], [2], z-transformation of the Maxwell curl equations [3], or the solution of an additional (auxiliary) differential equation between electric displacement density and polarization [4]–[8].

Recently, efforts have been undertaken to improve and optimize the efficiency with respect to computational effort and memory requirements of the different algorithms for handling of dispersive media, especially in the field of the recursive convolution (RC) and the auxiliary differential equation (ADE) methods. For the RC method, general algorithms can be derived that allow highly efficient simulation of any material with a complex electric permittivity that can be parametrized by means of a proper rational function of frequency. The accuracy can be influenced by using more or less exact algorithms for the numerical integration involved, which results in a trade-off between accuracy and computational efficiency. The ADE method, on the other hand, requires minor changes in the algorithm when modelling materials with different shapes of the permittivity function, i.e. different orders in the polynomials of the rational function. Straightforward implementation may lead to an unnecessary overhead in memory requirements and computation times. The big advantage over the RC methods, however, is the ADE methods' capa-

bility to handle nonlinear dispersive materials, which is not possible with RC due to the linearity intrinsic to the convolution integral.

We first present a new implementation of the ADE method for media with an arbitrary number of Lorentz relaxations [8]. In comparison to previously published formulations and implementations, more accurate results are obtained with this method, while it requires the same or less memory and fewer computational operations.

Our new formulation of the ADE method is then compared to three different implementations of the RC method. The first RC formulation examined uses the trapezoidal rule for the numerical evaluation of the convolution integral. It was presented in [9] and will be referred to as PLRC. The second scheme uses the quasi-trapezoidal approximation presented in [10], we will refer to it as QTRC method. The third method (CRC) is a reformulation of the algorithm presented in [6]. Though theoretically first-order in accuracy due to the use of the piecewise constant approximation in the evaluation of the convolution integral, this method also shows good accuracy in actual numerical experiments.

EFFICIENT ADE MODELLING OF LORENTZ MEDIA

We assume that we have a medium with a dispersive permittivity that can be characterized by N Lorentzian resonances. Each vector component of the electric displacement density D can be expressed in terms of electric field E and polarization P as

$$D(\vec{r}, t) = \epsilon_0 \epsilon_\infty E(\vec{r}, t) + P(\vec{r}, t) \quad (1)$$

It is further assumed that the polarization can be expressed as a sum of N terms for each of the resonances, i.e. $P = \sum_{i=1}^N P_i$ with each P_i being a convolution integral

$$P_i = \epsilon_0 \int_0^t \chi_i(t - \tau) E(\tau) d\tau \quad (2)$$

and $\chi_i(t)$ the Fourier transform of a Lorentzian in frequency

$$\chi_i(\omega) = \frac{g_i \omega_l^2 (\epsilon_s - \epsilon_\infty)}{\omega_l^2 + 2i\omega\delta_l - \omega^2} \quad (3)$$

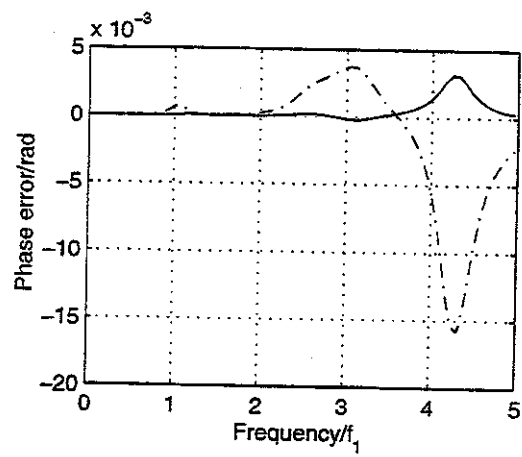
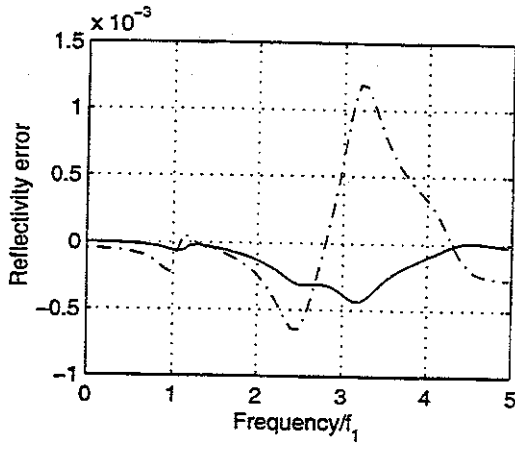


Figure 1: Comparison of ADE algorithms: Errors in the magnitude (left) and phase (right) of the reflection coefficient $\tau_{\text{analytical}} - \tau_{\text{FDTD}}$ as a function of frequency. The solid line was computed with the ADE algorithm presented in [8], and the dash-dotted curve was obtained using the algorithm described in [6].

with $\sum_{l=1}^N g_l = 1$. In the frequency domain we have

$$E(\omega) = \frac{\sum_{l=1}^N P_l}{\epsilon_0 \sum_{l=1}^N \chi_l} = \frac{D - \sum_{l=1}^N P_l}{\epsilon_0 \epsilon_\infty} = \frac{P_k}{\epsilon_0 \chi_k} \quad (4)$$

where $k = 1, \dots, N$. By Fourier transforming the right-most equality in (4), we obtain a system of coupled ordinary time domain differential equations

$$\ddot{P}_k + 2\delta_k \dot{P}_k + \omega_k^2 P_k = \omega_k^2 b_k (D - \sum_{l=1}^N P_l) \quad (5)$$

with $b_k = g_k(\epsilon_s - \epsilon_\infty)/\epsilon_\infty$ and $k = 1, \dots, N$.

The critical point for the efficiency and accuracy of the ADE algorithm is how the system of equations (5) is implemented numerically. In [6], a second-order accurate, semi-implicit central-difference scheme is used to update the polarization value. When using this scheme, one needs to store two previous values of each D component and two previous values for each P_k component ($k = 1, \dots, N$), i.e. a total of $2(N+1)$ old real values. In addition, an $(N \times N)$ by $(N \times 1)$ matrix-vector multiplication needs to be carried out, with the number of operations being proportional to N^2 . In [7], two improved schemes were reported which allow the solution of the auxiliary differential equation with reduced memory requirements ($2N$ and $2N+1$ real backstores in the formulations referred to as "LADEP" and "LADES", respectively) and computational effort ($10N$ and $12N$ operations (additions/multiplications), respectively).

We derive a new alternative scheme by discretizing (5) in the following way:

$$\begin{aligned} & (P_k^{n+1} - 2P_k^n + P_k^{n-1})/\Delta t^2 \\ & + \delta_k (P_k^{n+1} - P_k^{n-1})/\Delta t \\ & + \omega_k^2 P_k^n = \omega_k^2 b_k (D^n - \sum_{l=1}^N P_l^n) \end{aligned} \quad (6)$$

Solving for P_k^{n+1} gives an explicit updating scheme

$$P_k^{n+1} = a_{1,k} P_k^n + a_{2,k} P_k^{n-1} + a_{3,k} (D^n - \sum_{l=1}^N P_l^n) \quad (7)$$

where

$$\begin{aligned} a_{1,k} &= (2 - \omega_k^2 \Delta t^2)/(\delta_k \Delta t + 1) \\ a_{2,k} &= (\delta_k \Delta t - 1)/(\delta_k \Delta t + 1) \\ a_{3,k} &= \omega_k^2 \Delta t^2 b_k / (\delta_k \Delta t + 1) \end{aligned} \quad (8)$$

for $k = 1, \dots, N$ and Δt the time step. As for the complete electric field updating, the following steps have to be performed at each location for each field component:

$$\begin{aligned} D^{n+1} &= D^n + \Delta t \nabla \times \mathbf{H}^{n+\frac{1}{2}} \\ P_k^{n+1} &= a_{1,k} P_k^n + a_{2,k} P_k^{n-1} + a_{3,k} E^n \\ E^{n+1} &= (D^{n+1} - \sum_{l=1}^N P_l^{n+1})/(\epsilon_0 \epsilon_\infty), \end{aligned} \quad (9)$$

with k running through $1, \dots, N$ and $a_{4,k} = \epsilon_0 \epsilon_\infty a_{3,k}$.

Implementing the ADE method in the above way, a total of $6N+1$ operations (additions or multiplications) and memory for storage of $2N+1$ old values is required in addition to the standard FDTD algorithm for nondispersive materials.

NUMERICAL RESULTS

In order to evaluate the accuracy of the different algorithms, comparisons between FDTD and analytical results for a simple test example were carried out. For this purpose, we computed the frequency dependent reflection coefficient for a plane wave which impinges perpendicularly from vacuum onto a half plane filled with a dispersive medium. We assumed a highly dispersive material with two Lorentzian resonances, i.e.

Algorithm		Magnitude		Phase		Computation effort	
		Δ_{\max}	Δ_{rms}	Δ_{\max}/rad	$\Delta_{\text{rms}}/\text{rad}$	ops.	mem.
ADE	Hi-Res	4.4×10^{-4}	1.9×10^{-4}	3.2×10^{-3}	8.9×10^{-4}		
	Lo-Res	7.1×10^{-3}	3.0×10^{-3}	5.3×10^{-2}	1.5×10^{-2}	$6N + 1$	$2N + 1$
	Taflove	1.2×10^{-3}	4.3×10^{-3}	1.6×10^{-2}	4.5×10^{-3}	$> 2N^2 + 7N$	$2N + 2$
	LADEP	7.5×10^{-3}	2.8×10^{-3}	2.5×10^{-2}	6.0×10^{-3}	$10N$	$2N$
	LADES	1.9×10^{-3}	4.1×10^{-4}	5.0×10^{-3}	2.1×10^{-3}	$12N$	$2N + 1$
RC-HR	CRC	3.4×10^{-4}	1.4×10^{-4}	1.4×10^{-3}	4.5×10^{-4}	$8N - 2$	$2N$
	QTRC	2.9×10^{-4}	1.1×10^{-4}	4.4×10^{-3}	1.3×10^{-3}	$8N$	$2N$
	PLRC	3.1×10^{-4}	1.1×10^{-4}	2.3×10^{-3}	6.8×10^{-4}	$16N$	$2N + 1$
RC-LR	CRC	5.4×10^{-3}	2.2×10^{-3}	2.5×10^{-2}	7.8×10^{-3}	$8N - 2$	$2N$
	QTRC	4.6×10^{-3}	1.7×10^{-3}	6.8×10^{-2}	1.9×10^{-2}	$8N$	$2N$
	PLRC	5.0×10^{-3}	1.7×10^{-3}	3.4×10^{-2}	1.0×10^{-2}	$16N$	$2N + 1$

Table 1: Reflection coefficient error norms for a plane wave incident on a dispersive medium. “ops.” gives the number of operations, “mem.” the number of real storage space required per field component in addition to standard FDTD when simulating a medium with N Lorentzian resonances.

$N = 2$. The other parameters were $\epsilon_s = 3$, $\epsilon_\infty = 1.5$, $\omega_1 = 2\pi f_1$, $\omega_2 = 5\pi f_1$, $\delta_k = 0.1\omega_k$, ($k = 1, 2$), $g_1 = 0.4$ and $g_2 = 0.6$. The complex reflection coefficient r can be obtained analytically from the Fresnel formulae as $r(\omega) = (n(\omega) - 1)/(n(\omega) + 1)$, with the refractive index $n(\omega) = \sqrt{\epsilon(\omega)}$. Two sets of FDTD simulations with different grid spacings were carried out: For the high-resolution case we used a 1×2500 nodes grid with a time step $\Delta t = 400/f_1$ and grid spacing $d = c_0 \Delta t$, with c_0 the vacuum speed of light. For the low-resolution case modelling was done on a 1×625 nodes grid with a time step $\Delta t_{\text{LR}} = 4\Delta t$ and a node spacing $d_{\text{LR}} = 4d$. A Gaussian pulse plane wave excitation was introduced via a total field/scattered field boundary. The reflection coefficients were then computed numerically by Fourier transforming the reflected fields at the material interface and compared to the analytical results.

In the first part of our examination, accuracy and efficiency of the ADE formulations described above were compared. Fig. 1 shows the errors in the magnitude and phase of the electric field reflection coefficient for the ADE algorithm presented in [8] in comparison with the algorithm from [6]. Though requiring less memory and fewer computational operations, the new formulation leads to more accurate results. Comparison to Fig. 1 and Fig. 2 in [7] suggests that our algorithm is also superior to the ones presented there in terms of result accuracy. An overview the computational effort required and the accuracy of the results obtained is given in Table 1 (some of the figures are in correction of [8], where some mixing up occurred in the process of typesetting). “Hi-Res” and “Lo-Res” refer to the ADE algorithm presented here for the two resolution cases

described above. “Taflove” refers to the ADE formulation presented in [6], “LADEP” and “LADES” to algorithms presented in [7].

In the second part, we compared the various RC algorithms. Fig. 2 shows the reflection coefficient errors for the PLRC and QTRC algorithms, Fig. 3 the errors for the CRC algorithm. Again, Table 1 shows all the relevant data concerning accuracy and efficiency. “RC-HR” refers to the high resolution case, “RC-LR” to low resolution. Though theoretically of second order accuracy, the QTRC and PLRC formulations give only slightly more accurate results than the theoretically first order accurate CRC method, as far as reflection coefficient magnitude is concerned. Moreover, the CRC formulation gives significantly better results for the reflection coefficient phase. We believe, however, that the error in the phase is the less important measure due to the fact that the material interface is only localized to within the node distance in the FDTD grid. In addition, when modelling media with Debye relaxation behaviour [6], [7], numerical instabilities occurred for the CRC algorithm, especially when modelling the “muscle” media from [7]. We therefore believe that the QTRC formulation gives the best trade-off between accuracy, efficiency and numerical stability when modelling general, linear dispersive media.

Comparing ADE and RC methods shows that with the formulation presented in [8] the ADE methods can be implemented to perform with the same efficiency as the RC methods. Though for certain situations ($N = 1$) the CRC algorithm is in fact slightly more efficient, in all other cases the ADE is superior as far as the number of necessary operations is concerned, while requiring

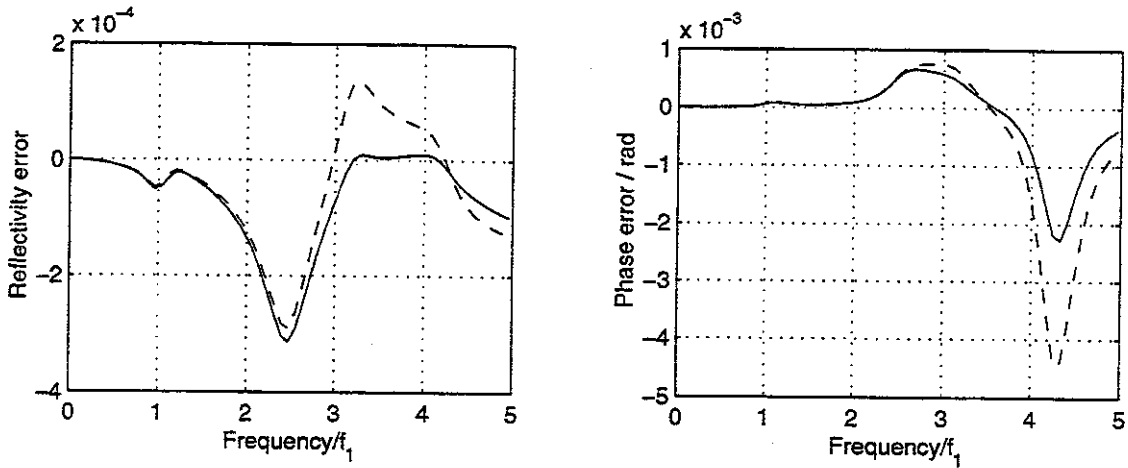


Figure 2: As in Fig. 1, but solid line: computed with the PLRC algorithm, dashed line: computed with the QTRC algorithm.

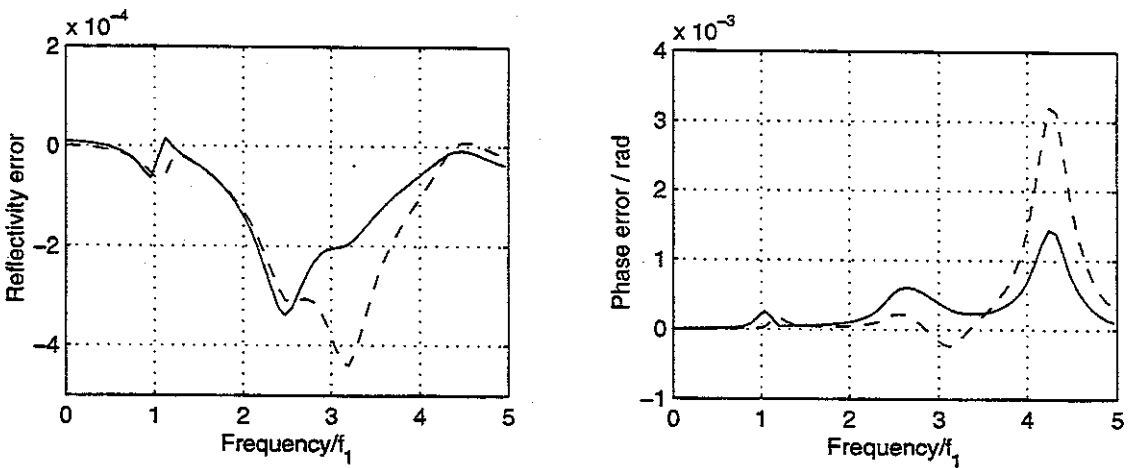


Figure 3: As in Fig. 1, but solid line: computed with the CRC algorithm, dashed line: computed with the ADE algorithm presented in [8].

slightly more memory than QTRC. The results that are obtained show very good agreement with analytical values, however, the RC methods perform even better with respect to accuracy.

Comparing the results for the two different grid resolutions in Table 1 shows that for all the formulations a fourfold increase in node spacing and time step leads to an approximately 16-fold increase in reflection coefficient magnitude error. Following the line of argumentation employed in [6], this suggests that all the algorithms presented here are practically second order accurate.

CONCLUSIONS

A new, efficient implementation of the Auxiliary Differential Equation method for treating dispersive media in finite-difference time-domain methods was presented. It requires fewer computational operations and comparable or less memory than previously published ADE and Recursive Convolution algorithms, especially for $N > 1$.

While the formulation gives more exact results than other ADE formulations, it does not achieve the accuracy of RC based methods. Since the latter are also capable of handling a variety of shape functions for the dielectric constant without modifications to the algorithm, they seem to be highly recommendable for modelling of general linear dispersive media.

ACKNOWLEDGEMENTS

This work was supported by the Swiss Commission for Technology and Innovation (KTI), project 3193.1.

REFERENCES

- [1] R. J. Luebbers, F. Hunsberger, K. S. Kunz, R. B. Standler, and M. Schneider. A frequency-dependent finite-difference time-domain formulation for dispersive materials. *IEEE Trans. Electromagn. Compat.*, 32(3):222–227, 1990.
- [2] R. Luebbers, D. Steich, and K. Kunz. FDTD calculation of scattering from frequency dependent materials. *IEEE Transactions on Antennas and Propagation*, 41(9):1249–1257, September 1993.
- [3] D. M. Sullivan. Frequency-dependent FDTD methods using Z transforms. *IEEE Transactions on Antennas and Propagation*, 40(10):1223–1230, October 1992.
- [4] R. M. Joseph et al. Direct time integration of Maxwell's equations in linear dispersive media with absorption for scattering and propagation of femtosecond electromagnetic pulses. *Optics Letters*, 16:1412–1414, 1991.
- [5] O. P. Gandhi, B. Q. Gao, and J. Y. Chen. A frequency-dependent finite-difference time-domain formulation for general dispersive media. *IEEE Trans. Microwave Theory Tech.*, 41(4):658–665, 1993.
- [6] A. Taflov. *Computational Electrodynamics — The Finite-Difference-Time-Domain Method*. Artech House, 1995.
- [7] M. Okoniewsky et al. Simple treatment of multi-term dispersion in FDTD. *IEEE Microwave and Guided Wave Letters*, 7(5):121–123, May 1997.
- [8] T. O. Körner and W. Fichtner. Auxiliary differential equation method: Efficient implementation in FDTD. *Optics Letters*, 22:1586–1588, 1997.
- [9] D. F. Kelley and R. J. Luebbers. The piecewise linear recursive convolution method for incorporating dispersive media into FDTD. In *11th Annual Review of Progress in Applied Computational Electromagnetics*, volume 1, pages 526–533, Monterey, CA, March 1995.
- [10] R. Siushansian and J. LoVetri. Efficient evaluation of convolution integrals arising in FDTD formulations of electromagnetic dispersive media. *J. Electromagn. Waves Applicat.*, 11(1):101–117, 1997.