Using Linear and Nonlinear Predictors to Improve the Computational Efficiency of the FD-TD Algorithm

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Abstract—It is well known that the Finite-Difference Time-Domain (FD-TD) method requires long computation times for solving electromagnetic problems, especially for high-Q structures. The reason for this is because the algorithm is based on the leap-frog formula. In this paper, both linear and nonlinear predictors, which are widely used in signal processing, are introduced to reduce the computation time of the FD-TD algorithm. A short segment of an FD-TD record is used to train the predictor. As long as the predictor is set up properly, an accurate future realization can be obtained. We demonstrate, by means of numerical results, that the efficiency of the FD-TD method can be improved by up to 90%. With this result, the FD-TD algorithm becomes a much more attractive technique for solving electromagnetic problems.

I. INTRODUCTION

THE finite-difference time-domain (FD-TD) method has been used widely for solving electromagnetic problems [1], [2]. It gives the evolution of the fields in time, given a known excitation. This leads to a complete understanding of near fields and of transient effects. Also, it is easily applied to problems composed of complex structures, which may be difficult to solve using other numerical methods. However, a major draw back of the FD-TD method is its computation time. In order to obtain accurate frequency responses via a Fourier transform, a very long time-domain record is usually needed. For some structures, especially those with high Q-values, the computation time may require up to a few days. Premature termination in the time domain will result in inaccurate parameter extraction in the frequency domain. To enhance the FD-TD method for simulating microwave problems, one begins by combining it with signal processing techniques such as the MUSIC method [3], or the System Identification (SI) method [4]. Both of these techniques can give accurate spectra using only a short segment of the original FD-TD record. However, up to now, these methods have only been used to predict the resonant frequency or spectrum of resonant structures. Another successful example of combining the FD-TD method with a signal processing technique, in order to reduce the computational overhead, is to use the FD-TD method with Prony's technique [5], [6]. In this combination, Prony's technique is used to predict the future realization of the time domain response by training a short segment of an FD-TD record and setting up coefficient-based

Manuscript received May 19, 1993; revised November 19, 1993.
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models, where the order is to be determined. Unfortunately, this method may require preknowledge to select the order of the coefficients for different structures [6]. Sometimes, it may be somewhat difficult to find the proper order. Even with these limitations, all of the above signal processing techniques can save computational time when using the FD-TD method to solve electromagnetic problems. It is very clear that the incorporation of signal processing techniques with the FD-TD method is an effective way to improve the efficiency of the FD-TD method. Once the FD-TD technique is formulated to solve a particular electromagnetic problem, the algorithm can be treated as a system, whose execution can be carried out using the appropriate signal processing technique. The fundamental operation of the FD-TD algorithm is based on the leap-frog formula, which means that future realizations are based on calculations that occurred in the past. In this paper, linear and nonlinear predictors are introduced, which can take advantage of the leap-frog nature of the FD-TD method to predict the later response of the system in the time domain. The following section gives detailed descriptions of the linear and nonlinear predictors used in this study. In Section III, some numerical results are given to show how these techniques are used to improve the efficiency of the FD-TD method. Conclusions and future work will be given in Section IV.

II. METHODOLOGY

A. General Description of the FD-TD Method

The FD-TD algorithm is a method in which the central difference scheme is used to discretize Maxwell's curl equations in both time and space. The central difference technique can contain the magnitude of the round-off errors so that second-order accuracy is achieved. To model the electrical and magnetic fields in space, Yee introduced the cell system in 1966 [7]. The physical basis for Yee's cell system can be easily explained using Faraday's and Ampere's laws. After using Yee's cell system to describe the computation domain, which is bounded by electric, magnetic or application specific absorbing walls, Maxwell's equations are essentially replaced by a computer which calculates the fields at the grid points associated with the cells.

In this paper, a Gaussian pulse, whose 3dB cut off frequency is designed to overlap with the frequency band of interest, is used as the excitation. The time step is given by

$$\Delta t = 0.5 \Delta h/c \tag{1}$$

where $\Delta h = \min\{\Delta x, \Delta y, \Delta z\}$. $\Delta x, \Delta y$ and Δz are the space steps in X, Y, and Z directions. c is the free-space velocity.

For a high dielectric constant material ($\varepsilon_r = 9.9$), the waves that propagate along the microstrip line are strongly dispersive. It is appropriate, therefore, that Litva's [8] dispersive boundary condition be used here. This boundary condition has been found to have very good performance with dispersive waves.

B. Linear Predictor

Linear predictors or autoregressive (AR) models have found applications in many fields of research [9]. It is the most popular time series modeling approach being used in modern spectral estimation [10]. This is because accurate estimation of the AR parameters can be derived by solving a set of linear equations. In contrast to Prony's method, which uses a model consisting of deterministic exponentials to fit the data, the AR model seeks a random model, to the second-order, to fit a statistical data base. Also, compared with the autoregressive moving average (ARMA) method, AR modeling does not require the solution of a set of highly nonlinear equations.

We say that the time series $x(n), x(n-1), \dots x(n-p)$ represents the realization of an autoregressive process of order p if it satisfies the equation,

$$x(n) = -a_1 x(n-1) - a_2 x(n-2) - \dots + a_p x(n-p) + \varepsilon$$
 (2)

where ε is an error term, and $a_1a_2,\ldots a_p$ are constants called the AR parameters. From equation (2), we see that the present value of the process u(n) is equal to a finite linear combination of past values of the process, $x(n-1), x(n-2), \ldots x(n-p)$, plus the error term $\varepsilon(n)$. Therefore, the present status can be predicted using a linear combination of previous observations. So, as long as the linear predictor is set up properly, through simple extrapolation, we can get the future realization.

There are two issues that must be addressed when setting up an AR model. One is how to choose the order of the model. The other is how to estimate the coefficients. The selection of the model order in AR is a critical problem. Using an order value which is too low results in a high rate of attenuation when extrapolating into the future, while too large an order causes general numerical instability. Two commonly used model order estimators are the final prediction error (FPE) technique and the Akaike Information Criterion (AIC)[10]. They are both based on the estimated predictor error power and are regarded as general guides for AR model selection. Although, the actual order which is selected in practice may be higher than the order given by these two techniques, at least, these two methods give a starting point for the selection of the order of the process. There are a large number of methods for estimating the AR parameters. In this paper, we choose the covariance method.

The covariance for AR parameter estimation yields the

solution of the equations,

$$\begin{bmatrix} c_{xx}(1,1) & c_{xx}(1,2) & \cdots & c_{xx}(1,p) \\ c_{xx}(2,1) & c_{xx}(2,2) & \cdots & c_{xx}(2,p) \\ \vdots & \vdots & \vdots & \vdots \\ c_{xx}(p,1) & c_{xx}(p,2) & \cdots & c_{xx}(p,p) \end{bmatrix} \begin{bmatrix} \hat{a}(1) \\ \hat{a}(2) \\ \vdots \\ \hat{a}(p) \end{bmatrix} = - \begin{bmatrix} c_{xx}(1,0) \\ c_{xx}(2,0) \\ \vdots \\ c_{xx}(p,0) \end{bmatrix}$$
(3)

where

$$c_{xx}(j,k) = \frac{1}{N-P} \sum_{n=p}^{N-1} x(n-j)x(n-k).$$
 (4)

The matrix is Hermitian and positive semidefinite. It can be solved by Cholesky decomposition. Under certain conditions [11], the solution of the AR parameters yields the following equations,

$$\begin{bmatrix} x(1) & x(2) & \cdots & x(p) \\ x(2) & x(3) & \cdots & x(p+1) \\ \vdots & \vdots & \vdots & \vdots \\ x(N) & x(N+1) & \cdots & x(p+N) \end{bmatrix} \begin{bmatrix} \hat{a_1} \\ \hat{a_2} \\ \vdots \\ \hat{a_p} \end{bmatrix}$$

$$= -\begin{bmatrix} x(p+1) \\ x(p+2) \\ \vdots \\ x(p+N) \end{bmatrix}. \tag{5}$$

Normally the value of N is chosen to be greater than 2p. Then the least-square algorithm is used to obtain the coefficients.

C. Nonlinear Predictor

The development of the upcoming class of nonlinear autoregressive models is motivated by the observation that many processes in nature display random variations which are essentially non-Gaussian in character [12]. In real world applications, it is found that many random processes display essentially nonlinear behavior and hence some form of nonlinear time series modeling, is required to accurately capture the process [13]. These nonlinear models are usually classified under the name of amplitude-dependent exponential autoregressive models. The basic form for an EXPAR(exponential autoregressive) model of order p is

$$x(t) = \sum_{j=1}^{p} [\alpha_j + \beta_j \exp(-\delta x^2 (t - j))] x(t - j) + \varepsilon_t \qquad \delta > 0$$
(6)

where ε_t is an error term. δ is a constant. α and β are the EXPAR parameters to be trained. Note that the above model contains no "constant terms" because Ozaki seems to take the view that "if the vibration process starts from the zero initiation state, it stays at zero" [14]. From (6), we can set up equations for the parameter δ as (7) shown at the bottom of the following page.

The equations are then solved using the least squares method. Also, in (7) we require N to be greater than 2p. Experimental evidence suggests that there can be difficulties with the estimation of δ , which is a critical parameter [13]. Since δ is essentially a scaling factor, it is reasonable to look

at values of δ in a range such that $e^{-\delta x_{t-i}^2}$ is different from both zero and equal to one for most values of x_{t-i} [12].

D. Discussion

There are three reasons for our introducing signal processing based models here. They are as follows:

- As we know, the FD-TD algorithm for electromagnetic simulation is a leap-frog algorithm, which means that the present value is iterated from a previously known value. When we look at the AR and EXPAR models, we find that they also predict their future values based on past occurrences. Since they both use the past to predict the future, this similarity prompts us to incorporate the AR and EXPAR models in the FD-TD algorithm, with a considerable saving in computation time.
- 2) It is well known in signal processing that a signal consisting of a number of sinusoids can be modeled using AR because of the recursive nature of this algorithm. When we use FD-TD to analyze high-Q structures, we rely on the fact that the time response can be approximated by a summation of sinusoidal waves. It follows that when high-Q structures are analyzed, an AR model can be used to provide an estimate of the future realization because of the similarity between the underlying basis functions for AR and high-Q structures. However, if there are some nonlinear effects in the system, we should add nonlinear terms to the model. Thus, for some cases, an EXPAR model is needed.
- 3) The classical problem in AR modeling is selecting of the correct order for the process. As mentioned earlier, there are two main tests that are used to determine order. However, in practice, they can't work perfectly all of the time. Normally we will choose a value for the order which is greater than that given by either PFE or AIC in order to be sure that the AR process adequately models the problem. Complex structures normally require high order models. It is found that on occasion the choice of a high order process leads to disastrous results in that the process fails to converge. We find that this conflict can be circumvented by using the EXPAR technique. Failure of convergence does not seem to be a problem when using this technique. In practice, when EXPAR is implemented, computational difficulties disappear.

III. NUMERICAL RESULTS

In this section, three typical electromagnetic problems are studied. They consist of two microwave filters and a patch antenna. The usefulness of AR and EXPAR modeling for improving the computational efficiency of FD-TD will be demonstrated.

Before one uses AR or EXPAR models to analyze FD-TD records, there are two issues that must be addressed. One is the selection of the segment of the FD-TD record to be used for training the AR or EXPAR models. The segment should cover a significant fraction of a FD-TD time record except for the very beginning of the FD-TD waveform. By avoiding the very beginning of the record, we ensure that the intricacies of the structure being analyzed are captured by the data used for training our model. For complex structures, we usually choose the beginning of the training segment to coincide with three times the round-trip time required for the launched pulse to be reflected from an extremity of the structure. The other requirement is that the original FD-TD records must undergo some decimation. To meet the FD-TD stability condition, the FD-TD algorithm usually oversamples the data compared to the needs of the AR and EXPAR models. If the oversampled FD-TD records were to be modeled without decimation, a very high order AR model would be required. This would lead to divergence between predicted and the true values. If we decimate the FD-TD records by a certain factor, the divergence of the predicted result is avoided. In real applications, the FD-TD records are usually decimated by a certain factor.

As our first example, AR modeling is applied to an edge coupled bandpass filter [15] as shown in Fig. 1. In order to obtain an accurate estimation of the S parameters, over 30000 iterations are needed if the original FD-TD method is used. By using the AR approach, only 2000–3500 iterations of the FD-TD algorithm are required to generate the original data base for the AR process, denoted as $\{u\}$. Decimating the $\{u\}$ by the factor 10, we get a time series $\{x\}$. Then $\{x\}$ is used to develop an AR model of order 50. Fig. 2 gives a comparison between the result obtained by FD-TD plus AR model and the direct FD-TD computation alone. It should be added that once the AR parameters are set up, the AR model can accurately predict very long time-domain traces of transient waveforms. Fig. 3 shows the S parameter calculated by the FD-TD plus AR model, and the direct FD-TD using 3500 FD-TD time

$$\begin{bmatrix} x(1) & x(2) & \cdots & x(p) & \exp(-\delta x^{2}(1)) & \exp(-\delta x^{2}(2)) & \cdots & \exp(-\delta x^{2}(p)) \\ x(2) & x(3) & \cdots & x(p+1) & \exp(-\delta x(2)) & \exp(-\delta x^{2}(3)) & \cdots & \exp(-\delta x^{2}(p+1)) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x(N) & x(N+1) & \cdots & x(p+N) & \exp(-\delta x^{2}(N)) & \exp(-\delta x^{2}(N+1)) & \cdots & \exp(-\delta x^{2}(p+N)) \end{bmatrix} \times \begin{bmatrix} \hat{a}_{2} \\ \vdots \\ \hat{a}_{p} \\ \hat{\beta}_{1} \\ \vdots \\ \hat{\beta}_{p} \end{bmatrix} = - \begin{bmatrix} x(p+1) \\ x(p+2) \\ \vdots \\ x(p+N) \end{bmatrix}$$

$$(7)$$

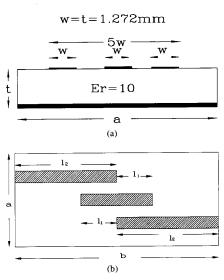


Fig. 1. (a) Plane of edged–coupled bandpass filter. (b) Cross–section of the filter. $l_1=6.36$ mm, $l_2=\frac{b}{2}=8.48$ mm, a=11.62 mm, w=t=1.272 mm, $\Delta x=\Delta y=\Delta z=\frac{w}{4}$.

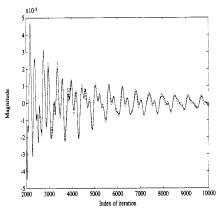


Fig. 2. AR result, composed of a short training segment, plus an extended extrapolated segment, all compared with a completed FD-TD data set.

domain iterations, as well as a measured result. It is observed that the result obtained using FD-TD plus the AR model agrees very well with the measured results.

The next example [16], is shown in Fig. 4. There we apply the proposed FD-TD plus AR model to a printed antenna. The AR model is based on a data set, which was generated during iterations 1200-2500 following the start of the FD-TD algorithm. Fig. 5 shows the AR extrapolation compared with FD-TD result. The values for the S parameter using FD-TD plus AR model are compared with measured data in Fig. 6.

The third example is the classical double-stub structure which is shown in Fig. 7 [17]. When analyzed using the FD-TD technique, this type of structure requires a large computational space, because the ratio of maximum to minimum dimensions of the structure is large. It also follows that the computational time is extremely long. So long, in fact, that it

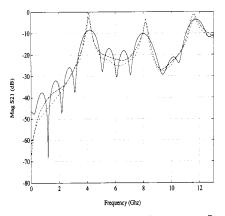


Fig. 3. Edged-coupled microstrip filter scattering parameter S_{21} .

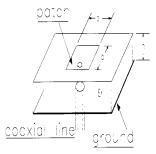


Fig. 4. Coaxial fed microstrip patch antenna,h=17.72 mm, b=25.1 mm, $\varepsilon_r=2.33,\ h=2.35$ mm, and feed point at (12.5, 4.0) mm, $\Delta x=\frac{h}{6},\ \Delta y=\Delta z=0.3125$ mm.

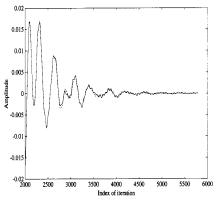


Fig. 5. AR curve fitting and extrapolation using patch antenna FD-TD records from 1200-2500.

is practically impossible to solve this problem using the FD-TD algorithm and conventional computing facilities. To start, we use the FD-TD technique and generate a data set of 8900 records. The data set is then decimated by a factor of 25. After that, a 91th order AR model is applied to get the coefficients using records for iteration 3100–8900. The predictor is then used to extend the data set out to 100000 iterations. The transmission coefficient coefficient is then obtained. Thus,

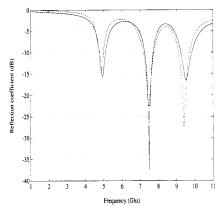


Fig. 6. Scattering parameter S_{11} of coaxial—fed patch antenna.

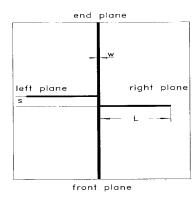


Fig. 7. Configuration of the double-stubstructure, w=0.1219 mm, L=2.921 mm, s=0.7569 mm, $\varepsilon_r=9.9$, h=12.7 mm, $\Delta x=\frac{h}{4}$, $\Delta y=\Delta z=\frac{w}{4}$.

based on a data set consisting of 100000 records, of which only 10% were obtained using the FD-TD algorithm, we have realized very good agreement with results obtained using a frequency domain technique. However, it is not as easy as the previous example to obtain the AR order for this structure. The results of AR modeling are very sensitive to the order used for the process. When we apply EXPAR to this structure and select the order to be 80, 90 even 100, we find that there is not much change in the predicted data set. On the other hand, it is easier to determine the order of EXPAR (see Fig. 8). This suggests that in practice, if the structure is complex, we simply select an relatively large value for the order of the process, without having to determine the order for each specific problem. However, this matter is still under investigation.

IV. CONCLUSION

We have used linear and nonlinear predictors to improve the computational efficiency of the FD-TD algorithm. The results show that for equal levels of accuracy, great savings can be realized in CPU time. In our current approach, we use a short FD-TD data segment for setting up the AR parameters and use a predictor to get the future realization. Then we extract S parameters by means of Fourier transforms. In the future,

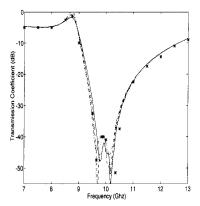


Fig. 8. Using EXPAR model to extract the transmission coefficient of the double-stub structure. $\delta=1.$

we expect to make a significant change in this procedure. We believe that once the model is set up, that the spectral information is contained in the coefficients. Instead of using a predictor which introduces errors into the result, it is thought that the S parameters can be extracted from the model itself as well as the initial data base. This work will make the system even faster and more accurate. Thus, the EM time-domain simulation technique will become more and more powerful.

ACKNOWLEDGMENT

The authors wish to thank Dr. Q. Wu, Ms. J. Li and Mr. Z. Hu at Communications Research Laboratory, McMaster University for their helpful discussion on this work. We would also wish to thank Sharon R. Aspden of Rogers Corp. for providing the dielectric material and information used in this research under the auspices of their university program. Finally, the authors acknowledge financial support provided by the Telecommunications Research Institute of Ontario.

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