Closed-Form Expressions for Coefficients Used in FD–TD High-Order Boundary Conditions

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Abstract— **Tirkas *et al.* recently presented an algorithm to implement absorbing boundary conditions (ABC's) of arbitrarily high order into the finite difference–time domain technique. However, they did not provide explicit formulas to determine the expansion coefficients used in the Padé approximations of the pseudo-differential operator. Instead, the user is required to determine the roots of a polynomial using numerical methods that require computational effort and yield only approximate results. Exact expressions for the desired coefficients that are valid for Padé expansions of any order are presented.**

I. Introduction

THE finite difference–time domain (FD–TD) method of electromagnetic analysis is a powerful and versatile technique which has become very popular in recent years. The method may be used to model structures with a high degree of inhomogeneity; also, the computational effort associated with FD–TD does not grow as rapidly with increasing structure size as it does for integral equation-based techniques. One of the difficulties in using FD–TD to analyze antennas and other structures in unbounded media is the need to terminate the computational grid. It is desirable to terminate the grid as close to the structure as possible in order to reduce the size of the computational domain and thus decrease the time and memory required to perform the analysis. However, the grid boundaries must be sufficiently distant from the scatterer so that the numerically implemented absorbing boundary condition (ABC) is effective in absorbing outgoing waves without significant reflection. Thus the quality of the ABC has a direct impact on the computational efficiency of an FD–TD code.

Most of the work in the area of improving the ABC has centered on accurately approximating the one-way wave equation operator. A comprehensive review of the relevant techniques can be found in [2]. Empirical numerical studies have shown that among the class of rational function approximations to the operator so far examined, Padé approximants yield the best results [1]. Thus it is important to have convenient formulas for implementing such approximations into the FD–TD formalism.

The authors of [1] presented a systematic method for implementing rational function ABC's by extending the approach of Lindman [3] to arbitrary order. However, they did not provide explicit formulas for the Lindman coefficients corresponding to a Padé approximation which are needed to actually implement the algorithm in a computer program. Without such formulas one must solve a system of linear equations for the standard Padé coefficients [4] and then employ a polynomial root-finding algorithm to determine the actual Lindman coefficients used in the ABC implementation. In place of this approximate procedure we offer simple, exact formulas in Section II and a proof of their correctness in Section III.

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II. Lindman Expansion Coefficients

We wish to approximate the two functions[1] $\sqrt{1-s^2}$ and $1/\sqrt{1-s^2}$ near $s=0$ by Lindman series of the form

$$L_M(s) = 1 - \sum_{m=1}^{M} \frac{a_m s^2}{1-b_m s^2}$$

and

$$K_M(s) = 1 + \sum_{m=1}^{M} \frac{c_m s^2}{1-d_m s^2},$$

respectively. The coefficients a_m, b_m, c_m, and d_m are required to implement high-order Padé ABC's and are uniquely determined by insisting that the first $4M+1$ derivatives at $s=0$ of $L_M(s)$ and $K_M(s)$ agree with those of $\sqrt{1-s^2}$ and $1/\sqrt{1-s^2}$, respectively.

The desired coefficients are given by the simple expressions

$$a_m = \frac{1}{2M+1}\left[1+\cos\frac{(2m-1)\pi}{2M+1}\right],$$
$$b_m = \frac{1}{2}\left[1-\cos\frac{(2m-1)\pi}{2M+1}\right],$$
$$c_m = a_m, \qquad d_m = 1-b_m,$$

for $m = 1,\cdots,M$.

III. Proof

We present the proof only for $\sqrt{1-s^2}$, since the proof for $1/\sqrt{1-s^2}$ is quite similar. We have the Maclaurin series expansion

$$\frac{1}{1-b_m s^2} = \sum_{n=0}^{\infty} b_m^n s^{2n}.$$

Also,

$$a_m = \frac{2}{2M+1}\cos^2\frac{(2m-1)\pi}{4M+2}, \quad b_m = \sin^2\frac{(2m-1)\pi}{4M+2}.$$

[1]When working in rectangular coordinates (as in [1]) only the expansion for $\sqrt{1-s^2}$ is required. The need for the expansion of $1/\sqrt{1-s^2}$ arises, for example, when solving the wave equation in a cylindrical coordinate system.

Thus, the first $2M+1$ nonzero terms of the Maclaurin series expansion of $L_M(s)$ are

$$\begin{aligned} S_M(s) &\equiv 1 - \frac{2}{2M+1} \sum_{m=1}^{M} s^2 \cos^2 \frac{(2m-1)\pi}{4M+2} \\ &\quad \cdot \sum_{n=0}^{2M-1} s^{2n} \sin^{2n} \frac{(2m-1)\pi}{4M+2} \\ &= 1 - \frac{2}{2M+1} \sum_{n=1}^{2M} s^{2n} \\ &\quad \cdot \sum_{m=1}^{M} \cos^2 \frac{(2m-1)\pi}{4m+2} \sin^{2n-2} \frac{(2m-1)\pi}{4M+2} \\ &= 1 - \frac{2}{2M+1} \sum_{n=1}^{2M} s^{2n} \left[\sum_{m=1}^{M} \sin^{2n-2} \frac{(2m-1)\pi}{4M+2} \right. \\ &\quad \left. - \sum_{m=1}^{M} \sin^{2n} \frac{(2m-1)\pi}{4M+2} \right]. \quad (1) \end{aligned}$$

By 1.320.1 of [5], we may write

$$\begin{aligned} &\sum_{m=1}^{M} \sin^{2n} \frac{(2m-1)\pi}{4M+2} \\ &= \sum_{m=1}^{M} \left\{ 2^{-2n} \left[\binom{2n}{n} + 2 \sum_{k=1}^{n} (-1)^k \binom{2n}{n-k} \right. \right. \\ &\quad \left. \left. \cdot \cos \frac{(2m-1)k\pi}{2M+1} \right] \right\} \\ &= \frac{2^{-n}(2n-1)!!\, M}{n!} + 2^{1-2n} \sum_{k=1}^{n} (-1)^k \binom{2n}{n-k} \\ &\quad \cdot \sum_{m=1}^{M} \cos \frac{(2m-1)k\pi}{2M+1}. \end{aligned}$$

However,

$$\begin{aligned} \sum_{m=1}^{M} \cos \frac{(2m-1)k\pi}{2M+1} &= \frac{\sin \frac{2kM\pi}{2M+1}}{2 \sin \frac{k\pi}{2M+1}} \\ &= \frac{\sin \left(k\pi - \frac{k\pi}{2M+1} \right)}{2 \sin \frac{k\pi}{2M+1}} = \frac{(-1)^{k-1}}{2}, \end{aligned}$$

for $1 \le k \le 2M$ by 1.342.4 of [5], so

$$\begin{aligned} &\sum_{m=1}^{M} \sin^{2n} \frac{(2m-1)\pi}{4M+2} \\ &\quad = \frac{(2n-1)!!\, M}{(2n)!!} - 2^{-2n} \sum_{k=1}^{n} \binom{2n}{n-k}, \end{aligned}$$

for $1 \le n \le 2M$. Also,

$$\begin{aligned} \sum_{k=1}^{n} \binom{2n}{n-k} &= \frac{1}{2} \left\{ \left[\sum_{k=0}^{2n} \binom{2n}{n} \right] - \binom{2n}{n} \right\} \\ &= \frac{1}{2} \left[2^{2n} - \frac{(2n)!}{(n!)^2} \right], \end{aligned}$$

so

$$\sum_{m=1}^{M} \sin^{2n} \frac{(2m-1)\pi}{4M+2} = \frac{(2n-1)!!\, M}{(2n)!!} - \frac{1}{2} + \frac{(2n-1)!!}{2^{n+1} n!}$$

and

$$\begin{aligned} &\sum_{m=1}^{M} \sin^{2n-2} \frac{(2m-1)\pi}{4M+2} - \sum_{m=1}^{M} \sin^{2n} \frac{(2m-1)\pi}{4M+2} \\ &= \frac{(2n-3)!!\, M}{(2n-2)!!} - \frac{1}{2} + \frac{(2n-3)!!}{2^n (n-1)!} \\ &\quad - \frac{(2n-1)!!\, M}{(2n)!!} + \frac{1}{2} - \frac{(2n-1)!!}{2^{n+1} n!} \\ &= \left[\frac{(2n-3)!!\, 2n - (2n-1)!!}{(2n)!!} \right] M \\ &\quad + \frac{(2n-3)!!\, 2n - (2n-1)!!}{2^{n+1} n!} \\ &= \frac{(2n-3)!!}{(2n)!!} M + \frac{1}{2} \frac{(2n-3)!!}{(2n)!!} \\ &= \frac{(2n-3)!!}{(2n)!!} \left(\frac{2M+1}{2} \right), \end{aligned} \quad (2)$$

for $1 \le n \le 2M$. Putting (2) in (1) yields

$$S_M(s) = 1 - \sum_{n=1}^{2M} \frac{(2n-3)!!}{(2n)!!} s^{2n}.$$

From the Maclaurin series expansion

$$\sqrt{1-s^2} = 1 - \sum_{n=1}^{\infty} \frac{(2n-3)!!}{(2n)!!} s^{2n},$$

we see that the first $4M+1$ derivatives of $\sqrt{1-s^2}$ and $L_M(s)$ are indeed equal.

IV. Conclusion

This letter presents closed-form formulas for the coefficients needed to implement Padé ABC's of arbitrarily high order. They are useful in constructing FD–TD computer programs of greater flexibility and accuracy than was previously possible.

References

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