Corrected Impulse Invariance Method in Z-Transform Theory for Frequency-Dependent FDTD Methods

Ding Yu Heh, *Student Member, IEEE*, and Eng Leong Tan, *Senior Member, IEEE*

***Abstract*—The classical impulse invariance method in Z-transform theory had been found to be incorrect and inaccurate when the impulse response is discontinuous at intial time $t = 0$. Such inaccuracy results in higher numerical errors if it is used to develop the update equations for frequency-dependent finite-difference time-domain (FDTD) methods. In this paper, thorough discussions of corrected impulse invariance method in the realm of Z-transform theory for dispersive media are presented. The correction is shown to be necessary for dispersive media which exhibit discontinuity at $t = 0$ in the time domain susceptibility function. A (corrected) Z-transform table is provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations of frequency-dependent FDTD update equations using both corrected and classical impulse invariance methods are carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements are included along with some extensive numerical comparisons.**

***Index Terms*—Corrected impulse invariance method, dispersive media, finite-difference time-domain (FDTD) method, Z-transform theory.**

I. Introduction

Over the years, there had been numerous efforts carried out to extend the Yee's finite-difference time-domain (FDTD) method for frequency-dependent media. Among these efforts, one approach is the Auxiliary Differential Equation (ADE) method (or Direct Integration method) [1]-[5], which converts the frequency-dependent Maxwell equations into auxiliary differential equations in time domain. An alternative approach is by discretizing the convolution integral relating the D and E fields, which results in Recursive Convolution (RC) method [6], [7] and Piecewise Linear Recursive Convolution (PLRC) method [8], [9]. In [10], [11], a Z-transform method was proposed which converts the transfer function in frequency domain into Z domain via a table of conversion. With this approach, the update equations can be obtained much more conveniently than the RC and PLRC methods. On the other hand, the Z-transform method in [12], [13] utilizes a single pole conductivity model to incorporate the dispersive effect of material under consideration. This is a distinct method that is not based on frequency domain but Z domain transfer function directly, and thus it will not be considered further in this paper. Reference [14] provided a review of methods for solving electromagnetic problems in dispersive (complex) media.

The Z-transform method of [10], [11] is in fact the classical impulse invariance method widely used in digital IIR filter design. This method, however, is incorrect and inaccurate when the impulse response is discontinuous at initial time $t = 0$. The problem had been highlighted in [15], [16] along with the necessary correction for it. Therefore, if classical impulse invariance method is to be used without any correction to formulate the frequency-dependent FDTD update equations, the overall accuracy of the computed electric and magnetic fields would be affected. It had been previously demonstrated in [17] that using the corrected impulse invariance method to model dispersive media would achieve an improved accuracy to the calculated electric fields. In this paper, we present the thorough discussions of corrected impulse invariance method in the realm of Z transform theory for dispersive media. A Z-transform table is provided to supplement and *correct* those Z-transform tables provided in [10], [11]. With the aid of the table, various formulations of frequency-dependent FDTD update equations are carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements are included along with some extensive numerical comparisons.

The organization of this paper is as follows. Section II describes the necessary correction needed for the classical impulse invariance method in Z-transform theory. A (corrected) Z-transform table is provided in this section to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations of the frequency-dependent FDTD update equations are detailed in Section III for Debye media. The memory storage requirements for all these methods are tabulated and compared. Section IV presents the complex numerical permittivities of all relevant methods, which are useful not only in studying the dispersion relation, but also in analyzing the order of temporal accuracy of various methods. Extensive numerical comparisons of various methods in terms of normalized phase, attenuation and numerical FDTD errors are then made in Section V.

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The authors are with the School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798 (e-mail: hehd0002@ntu.edu.sg; eeltan@ntu.edu.sg).

II. Z-Transform and Corrected Impulse Invariance

The relationship between a continuous time input $x(t)$ and output $y(t)$ is often described in frequency domain as

$$\widetilde{Y}(\omega) = \widetilde{H}(\omega)\widetilde{X}(\omega) \tag{1}$$

where $\widetilde{H}(\omega)$ is the transfer function of the system in frequency domain.The Z-transform will find much usefulness for obtaining the discrete time samples of the output $y(t)$ if we can specify the relationship between the input and output in Z domain such that

$$\widetilde{Y}(z) = \widetilde{H}(z)\widetilde{X}(z) \tag{2}$$

The question which remains is how to convert $\widetilde{H}(\omega)$ into $\widetilde{H}(z)$ accurately. To this end, by applying the frequency shifting property of the Fourier transform to the Poisson summation formula, it can be shown that

$$\sum_{n=-\infty}^{\infty} h(n\Delta t)e^{-j\omega n} = \frac{1}{\Delta t}\sum_{k=-\infty}^{\infty}\widetilde{H}\left(\frac{\omega-2\pi k}{\Delta t}\right) \tag{3}$$

where $h(t)$ is the impulse response and Δt is the time step or sampling period. Equation (3) indicates that the sampling process of a continuous time signal will produce multiple copies of its own Fourier transform periodically. It can be further recognized that the left hand side of (3) is exactly the discrete time Fourier transform of the sampled impulse response $h[n]$ or more importantly, its Z-transform evaluated on the unit circle of Z plane. Thus, the relationship between the frequency and Z domains of a function is established and governed by (3).

In frequency-dependent FDTD schemes, the analogy to the systems described in (1) and (2) are in two folds. Firstly, the electric and magnetic fields are related to their respective flux densities by frequency-dependent permittivity and permeability. Secondly, the FDTD operates in a discrete time scheme. In [10] and [11], the author made use of the classical impulse invariance method, which unfortunately, is inaccurate when the (causal) impulse response $h(t)$ of the media is discontinuous at initial time $t=0$ [15], [16]. The crux of the inaccuracy lies in the inappropriately chosen value of the discrete $h[0]$, where it is directly assumed from the initial value theorem as $h(0^+)$. The consequence is that the Z-transform of $h[n]$ violates (3) under such circumstances. To avoid this violation, correction is therefore needed for the original classical impulse invariance method.

For more clarity, consider a causal exponentially decaying impulse response $e^{-\alpha t}u(t)$ where $u(t)$ is the unit step function. Note that this exponentially decaying impulse response has discontinuity at $t=0$ and the initial value theorem specifies that $h(0^+)$ equals one, which renders the classical impulse invariance method to choose $h[0]$ erroneously as unity. To find the correct value of $h[0]$ such that (3) is satisfied, we can further examine from (3) that $h[0]$ is nothing more than the Fourier series coefficient of $\sum_{k=-\infty}^{\infty}\frac{1}{\Delta t}\widetilde{H}\left(\frac{\omega-2\pi k}{\Delta t}\right)$ at $n=0$. Recognizing that the Fourier transform of $e^{-\alpha t}u(t)$ is $\widetilde{H}(\omega)=\frac{1}{j\omega+\alpha}$, we can write

$$h[0] = \frac{1}{2\pi}\int_0^{2\pi}\sum_{k=-\infty}^{\infty}\frac{1}{\Delta t}\frac{1}{\frac{j(\omega-2\pi k)}{\Delta t}+\alpha}d\omega \tag{4}$$

Upon some manipulations, we have

$$\begin{aligned}&\frac{1}{2\pi}\int_0^{2\pi}\sum_{k=-\infty}^{\infty}\frac{1}{\Delta t}\frac{1}{\frac{j(\omega-2\pi k)}{\Delta t}+\alpha}d\omega\\ &=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{j\omega+\alpha\Delta t}d\omega\end{aligned} \tag{5}$$

The value of $h[0]$ is finally determined as

$$h[0] = \lim_{\nu\to\infty}\frac{1}{\pi}\tan^{-1}\left(\frac{\nu}{\alpha\Delta t}\right) = \frac{1}{2} \tag{6}$$

Note that for convergence of (3), $\alpha > 0$ and $h[0]$ is only half the value as it was previously assumed using the classical impulse invariance method. This must be taken into consideration when Z-transform is performed on $h[n]$. Essentially, if the Z-transform is weighted with Δt (as in the classical impulse invariance method), subtraction of $\frac{\Delta t}{2}$ must be made to it.

For other forms of impulse response, a table of conversion among time, frequency and Z domains is provided, c.f. Table I. The entries for classical impulse invariance method used in [10], [11] and corrected impulse invariance method are included together for direct comparison. It should be noted that the Z domain is weighted with the time step, Δt. For the time domain dirac delta function, no weighing of Δt is required on its frequency and Z domains. Both classical and corrected impulse invariance methods directly inherit unity from the frequency domain to preserve the linearity property of the Fourier and Z transforms. For all the other entries, their Z domains obtained using the corrected impulse invariance method have been properly corrected. The correction needed is the subtraction of $\frac{\Delta t}{2}$ to their original Z domain obtained using the classical impulse invariance method. Alternatively, the subtraction can also be viewed as inclusion of an additional zero with opposite polarity to the pole of the Z domain transfer function.

In fact, all the corrections tabulated in Table I can be further justified by reusing the exponentially decaying impulse response described earlier to find their respective $h[0]$. For unit time step $u(t)$, we can find its $h[0]$ by letting α in (4) to be vanishingly small. It follows from (6) that $h[0]$ is also half instead of unity assumed by the classical impulse invariance method. For the time derivative of exponentially decaying impulse response, we can rewrite the frequency domain transfer function as $\frac{j\omega}{j\omega+\alpha}=1-\frac{\alpha}{j\omega+\alpha}$ and obtain the Z domain transfer function readily. The last two entries belong to the second order pole transfer function. With the aid of complex conjugate splitting, the value of $h[0]$ can still be determined conveniently. For the exponentially decaying

TABLE I
CONVERSION AMONG TIME, FREQUENCY AND Z DOMAINS

Time Domain	Frequency Domain	Z Domain (classical impulse invariance)	Z Domain (corrected impulse invariance)
$\delta(t)$	1	1	1
$u(t)$	$\frac{1}{j\omega}$	$\frac{\Delta t}{1-z^{-1}}$	$\frac{\Delta t}{2}\left(\frac{1+z^{-1}}{1-z^{-1}}\right)$
$e^{-\alpha t}u(t)$	$\frac{1}{j\omega+\alpha}$	$\frac{\Delta t}{1-e^{-\alpha\Delta t}z^{-1}}$	$\frac{\Delta t}{2}\left(\frac{1+e^{-\alpha\Delta t}z^{-1}}{1-e^{-\alpha\Delta t}z^{-1}}\right)$
$\frac{\partial}{\partial t}\left(e^{-\alpha t}u(t)\right)$	$\frac{j\omega}{j\omega+\alpha}$	$1-\frac{\alpha\Delta t}{1-e^{-\alpha\Delta t}z^{-1}}$	$1-\frac{\alpha\Delta t}{2}\left(\frac{1+e^{-\alpha\Delta t}z^{-1}}{1-e^{-\alpha\Delta t}z^{-1}}\right)$
$e^{-\alpha t}\cos(\beta t)\,u(t)$	$\frac{\alpha+j\omega}{\alpha^2+\beta^2+2\alpha j\omega-\omega^2}$	$\frac{\Delta t\left(1-e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}\right)}{1-2e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}+e^{-2\alpha\Delta t}z^{-2}}$	$\frac{\Delta t\left(1-e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}\right)}{1-2e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}+e^{-2\alpha\Delta t}z^{-2}}-\frac{\Delta t}{2}$
$e^{-\alpha t}\sin(\beta t)\,u(t)$	$\frac{\beta}{\alpha^2+\beta^2+2\alpha j\omega-\omega^2}$	$\frac{\Delta t e^{-\alpha\Delta t}\sin(\beta\Delta t)z^{-1}}{1-2e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}+e^{-2\alpha\Delta t}z^{-2}}$	$\frac{\Delta t e^{-\alpha\Delta t}\sin(\beta\Delta t)z^{-1}}{1-2e^{-\alpha\Delta t}\cos(\beta\Delta t)z^{-1}+e^{-2\alpha\Delta t}z^{-2}}$

cosine impulse response, it can be shown that

$$h[0]=\lim_{\nu\to\infty}\left[\frac{1}{2\pi}\tan^{-1}\left(\frac{\nu}{p\Delta t}\right)+\frac{1}{2\pi}\tan^{-1}\left(\frac{\nu}{p^*\Delta t}\right)\right]=\frac{1}{2} \tag{7}$$

where $p=\alpha+j\beta$. Again, $h[0]$ is only half as opposed to unity assumed by the classical impulse invariance method. Finally, for the exponentially decaying sine impulse response, its value of $h[0]$ can be shown as

$$h[0]=\lim_{\nu\to\infty}\left[\frac{j}{2\pi}\tan^{-1}\left(\frac{\nu}{p\Delta t}\right)-\frac{j}{2\pi}\tan^{-1}\left(\frac{\nu}{p^*\Delta t}\right)\right]=0 \tag{8}$$

In this case, $h[0]$ is found to be zero. Therefore, the impulse response is not discontinuous at $t=0$, and no further subtraction of $\frac{\Delta t}{2}$ is needed for its Z domain transfer function obtained using the classical impulse invariance method.

Notably, the (first order) exponentially decaying impulse response represents the form of time domain susceptibility function of a Debye medium. In the following, we will present various formulations for Debye media using the corrected impulse invariance method.

III. FORMULATIONS FOR DEBYE MEDIA

For a Debye medium having multiple first order poles, the complex relative permittivity is characterized by

$$\epsilon(\omega)=\epsilon_\infty+\sum_p\frac{A_p\Delta\epsilon}{1+j\omega\tau_p} \tag{9}$$

where $\Delta\epsilon=\epsilon_s-\epsilon_\infty$, ϵ_s is the static or zero-frequency relative permittivity, ϵ_∞ is the relative permittivity at infinite frequency, A_p is the p-th pole amplitude, and τ_p is the p-th pole relaxation time. It should be noted that the time domain impulse response of (9) is discontinuous at $t=0$. In the following subsections, the formulations from three different relations using both corrected and classical impulse invariance methods will be shown, along with their respective memory storage requirements. With the help of Table I, the conversion from frequency to Z domain can be done conveniently. The update equations in time domain can then be easily obtained from the Z domain equations by recognizing that the z^{-1} operator denotes the value at one time step earlier.

A. Formulation from D and E relation

The dependency between two phasors $\widetilde{\boldsymbol{D}}$ and $\widetilde{\boldsymbol{E}}$ is given by

$$\widetilde{\boldsymbol{D}}(\omega)=\left(\epsilon_0\epsilon_\infty+\sum_p\frac{\epsilon_0A_p\Delta\epsilon}{1+j\omega\tau_p}+\frac{\sigma}{j\omega}\right)\widetilde{\boldsymbol{E}}(\omega) \tag{10}$$

where ϵ_0 is the permittivity of free space and the conductivity, σ has also been included. Following the procedures in [17], the set of time domain update equations are

$$\boldsymbol{D}^{n+1}=\boldsymbol{D}^n+\Delta t\boldsymbol{\nabla}\times\boldsymbol{H}^{n+\frac{1}{2}} \tag{11a}$$

$$\boldsymbol{E}^{n+1}=\frac{\boldsymbol{D}^{n+1}-\sum_p\boldsymbol{S}_p^n-\boldsymbol{I}^n}{\epsilon_0\epsilon_\infty+\sum_p\frac{\epsilon_0A_p\Delta\epsilon\Delta t}{2\tau_p}+\frac{\sigma\Delta t}{2}} \tag{11b}$$

$$\boldsymbol{S}_p^{n+1}=\frac{\epsilon_0A_p\Delta\epsilon\Delta t}{\tau_p}e^{-\frac{\Delta t}{\tau_p}}\boldsymbol{E}^{n+1}+e^{-\frac{\Delta t}{\tau_p}}\boldsymbol{S}_p^n \tag{11c}$$

$$\boldsymbol{I}^{n+1}=\sigma\Delta t\boldsymbol{E}^{n+1}+\boldsymbol{I}^n \tag{11d}$$

It is reminded that the H fields are still updated as in conventional Yee's FDTD scheme throughout.

For comparison, invoking only the classical impulse invariance method [10], [11] to (10) will replace (11b) by

$$\boldsymbol{E}^{n+1}=\frac{\boldsymbol{D}^{n+1}-\sum_p\boldsymbol{S}_p^n-\boldsymbol{I}^n}{\epsilon_0\epsilon_\infty+\sum_p\frac{\epsilon_0A_p\Delta\epsilon\Delta t}{\tau_p}+\sigma\Delta t} \tag{12}$$

with the rest of (11) remain unchanged. Hereby, we point out that the difference posed by the corrected version compared to the classical impulse invariance method lies in the denominator terms of (12). For these two methods that originate from the relation between D and E , we shall refer to the corrected impulse invariance method as DE_{cor} and its classical impulse invariance method counterpart only as DE.

B. Formulation from P and E relation

The formulation in this subsection makes use of another relation described by

$$\widetilde{\boldsymbol{P}}_p(\omega) = \frac{\epsilon_0 A_p \Delta\epsilon}{1 + j\omega\tau_p}\widetilde{\boldsymbol{E}}(\omega) \tag{13}$$

where $\boldsymbol{P}$ (without tilde in time domain) is associated to Ampere's law as

$$\nabla \times \boldsymbol{H} = \epsilon_0\epsilon_\infty \frac{\partial}{\partial t}\boldsymbol{E} + \sigma\boldsymbol{E} + \sum_p \frac{\partial}{\partial t}\boldsymbol{P}_p \tag{14}$$

Invoking corrected impulse invariance method, and further combination with central difference approximation and time averaging of Ampere's law, one gets the final update equations as

$$\begin{aligned}\boldsymbol{E}^{n+1} =& c_1^{PE}\boldsymbol{E}^n + c_2^{PE}\Bigg(\nabla \times \boldsymbol{H}^{n+\frac{1}{2}} \\ & - \frac{1}{\Delta t}\sum_p \left(a_{1p}^{PE} - 1\right)\boldsymbol{P}_p^{n+1}\Bigg)\end{aligned} \tag{15a}$$

$$\boldsymbol{P}_p^{n+1} = a_{1p}^{PE}\boldsymbol{P}_p^n + a_{2p}^{PE}\boldsymbol{E}^{n+1} + a_{3p}^{PE}\boldsymbol{E}^n \tag{15b}$$

where

$$\begin{aligned} c_1^{PE} &= \left(\frac{2\epsilon_0\epsilon_\infty - 2\sum_p a_{3p}^{PE} - \sigma\Delta t}{2\epsilon_0\epsilon_\infty + 2\sum_p a_{2p}^{PE} + \sigma\Delta t}\right) \\ c_2^{PE} &= \left(\frac{2\Delta t}{2\epsilon_0\epsilon_\infty + 2\sum_p a_{2p}^{PE} + \sigma\Delta t}\right) \\ a_{1p}^{PE} &= e^{-\frac{\Delta t}{\tau_p}} \\ a_{2p}^{PE} &= \epsilon_0 A_p \Delta\epsilon \Delta t / 2\tau_p \\ a_{3p}^{PE} &= a_{1p}^{PE} a_{2p}^{PE} \end{aligned}$$

On the other hand, the final update equations resulting from classical impulse invariance method have the same form as (15a)-(15b), but with the following update coefficients replaced

$$\begin{aligned} a_{2p}^{PE} &= \epsilon_0 A_p \Delta\epsilon\Delta t/\tau_p \\ a_{3p}^{PE} &= 0 \end{aligned}$$

For these two methods that originate from the relation between P and E, we shall refer to the corrected impulse invariance method as PE_{cor} and its classical impulse invariance method counterpart only as PE.

C. Formulation from J and E relation

Alternatively, there exists another relation of the form

$$\widetilde{\boldsymbol{J}}_p(\omega) = \frac{j\omega\epsilon_0 A_p \Delta\epsilon}{1 + j\omega\tau_p}\widetilde{\boldsymbol{E}}(\omega) \tag{16}$$

where $\boldsymbol{J}$ is associated to Ampere's law as

$$\nabla \times \boldsymbol{H} = \epsilon_0\epsilon_\infty \frac{\partial}{\partial t}\boldsymbol{E} + \sigma\boldsymbol{E} + \sum_p \boldsymbol{J}_p \tag{17}$$

Similarly, invoking corrected impulse invariance method to (16) and further combination with central difference approximation and time averaging of Ampere's law, one gets the final update equations as

$$\begin{aligned}\boldsymbol{E}^{n+1} =& c_1^{JE}\boldsymbol{E}^n + c_2^{JE}\Bigg(\nabla \times \boldsymbol{H}^{n+\frac{1}{2}} \\ & - \frac{1}{2}\sum_p \left(a_{1p}^{JE} + 1\right)\boldsymbol{J}_p^{n+1}\Bigg)\end{aligned} \tag{18a}$$

$$\boldsymbol{J}_p^{n+1} = a_{1p}^{JE}\boldsymbol{J}_p^n + a_{2p}^{JE}\boldsymbol{E}^{n+1} + a_{3p}^{JE}\boldsymbol{E}^n \tag{18b}$$

where

$$\begin{aligned} c_1^{JE} &= \left(\frac{2\epsilon_0\epsilon_\infty - \Delta t\sum_p a_{3p}^{JE} - \sigma\Delta t}{2\epsilon_0\epsilon_\infty + \Delta t\sum_p a_{2p}^{JE} + \sigma\Delta t}\right) \\ c_2^{JE} &= \left(\frac{2\Delta t}{2\epsilon_0\epsilon_\infty + \Delta t\sum_p a_{2p}^{JE} + \sigma\Delta t}\right) \\ a_{1p}^{JE} &= e^{-\frac{\Delta t}{\tau_p}} \\ a_{2p}^{JE} &= \frac{\epsilon_0 A_p \Delta\epsilon}{\tau_p}\left(1 - \frac{\Delta t}{2\tau_p}\right) \\ a_{3p}^{JE} &= -a_{1p}^{JE}\frac{\epsilon_0 A_p \Delta\epsilon}{\tau_p}\left(1 + \frac{\Delta t}{2\tau_p}\right) \end{aligned}$$

The formulated final update equations from classical impulse invariance method will differ from (18a)-(18b) in terms of update coefficients given as

$$\begin{aligned} a_{2p}^{JE} &= \frac{\epsilon_0 A_p \Delta\epsilon}{\tau_p}\left(1 - \frac{\Delta t}{\tau_p}\right) \\ a_{3p}^{JE} &= -a_{1p}^{JE}\frac{\epsilon_0 A_p \Delta\epsilon}{\tau_p} \end{aligned}$$

For these two methods that originate from the relation between J and E, we shall refer to the corrected impulse invariance method as JE_{cor} and its classical impulse invariance method counterpart only as JE.

D. Memory Storage Requirements

The memory storage requirements for frequency-dependent FDTD methods is larger than that of a standard Yee's FDTD method for nondispersive media due to the need for additional auxiliary variables apart from E and H main field components. Tables II shows the amount of memory storage per cell needed in Debye media. N_e and N_h are the number of electric and magnetic field components respectively, and N_p is the number of dispersion term used to model a particular dispersive medium. N_e and N_h are dictated by the problem dimension and N_p is specified as to how well a Debye model fits a particular medium's frequency-dependent permittivity (based on nonlinear least square analysis [18]). The entries for ADE [4] and PLRC [8] methods are also included for comparison.

From Table II, it is clear that DE_{cor} [17] and DE [10], [11] require larger memory storage than the others because their formulations involve more variables. By simply redefining the auxilliary variables, we can achieve lower memory requirements. In particular, PE_{cor} and JE_{cor} are of great interest because they represent the corrected versions of all

TABLE II
MEMORY STORAGE REQUIREMENTS FOR DEBYE MEDIA

Method	Memory per Cell
DE_{cor}, DE	$2\ N_e + N_h + N_e N_p$
$PE_{cor}, PE,$ $JE_{cor}, JE,$ $ADE, PLRC$	$N_e + N_h + N_e N_p$

the Z-transform schemes and they still retain the storage requirements as in the case of ADE and PLRC methods. For large 3D problems, such savings in memory usage compared to DE_{cor} and DE are often desirable.

IV. DISPERSION RELATION AND COMPLEX NUMERICAL PERMITTIVITY

Using Fourier analysis in conjunction with central difference on Yee's cell, the frequency-dependent FDTD update equations can be represented as

$$-j\boldsymbol{K} \times \boldsymbol{H}_0 = j\Omega\epsilon_{nc}\boldsymbol{E}_0 \tag{19a}$$
$$-j\boldsymbol{K} \times \boldsymbol{E}_0 = j\Omega\mu_{nc}\boldsymbol{H}_0 \tag{19b}$$

where

$$\Omega = 2\sin\left(\omega\Delta t/2\right)/\Delta t$$
$$\boldsymbol{K} = K_x\hat{\boldsymbol{x}} + K_y\hat{\boldsymbol{y}} + K_z\hat{\boldsymbol{z}}$$
$$K_\xi = 2\sin\left(k_\xi\Delta\xi/2\right)/\Delta\xi$$

ϵ_{nc} and μ_{nc} are the complex numerical permittivity and permeability. For Yee's FDTD compatible methods, the update equations can be conveniently described in the form of (19a)-(19b), with ϵ_{nc} and μ_{nc} varying according to the type of material and the particular modeling method. From (19a)-(19b), we are also able to see that $\boldsymbol{K}\cdot\boldsymbol{E}_0 = 0$ and $\boldsymbol{K}\cdot\boldsymbol{H}_0 = 0$, which are indications of Yee's FDTD divergence-free nature [19]. The dispersion relation can then be derived from (19a)-(19b) as

$$\boldsymbol{K}\cdot\boldsymbol{K} = \Omega^2\mu_{nc}\epsilon_{nc} \tag{20}$$

For nondispersive, lossless media, ϵ_{nc} and μ_{nc} are constant values and (20) is reduced to dispersion relation of standard Yee's FDTD scheme. Since we only consider nonmagnetic materials here, μ_{nc} is assumed to be permeability of free space μ_0. Extension into dispersive magnetic materials is also possible and very straight forward. It can be seen that (20) describes the dispersion relation of a particular frequency-dependent FDTD method which is inherent from the complex numerical permittivity. Table III shows the list of complex numerical permittivity ϵ_{nc} of various Z-transform methods for Debye media. The leading error term of the complex numerical permittivity is the error term with the lowest order of Δt, obtained by performing Taylor series expansion of ϵ_{nc} and comparing to the analytical $\epsilon(\omega)$. Also shown in the table are the entries of ADE and PLRC methods for comparison. For other variations of direct integration and recursive convolution methods, readers can refer to [20].

Looking at Table III, it is observed that all corrected impulse invariance methods for Debye media have leading error terms of one order higher than all classical impulse invariance methods with respect to Δt. This implies that corrected impulse invariance method indeed has temporal accuracy of one order higher than classical impulse invariance method. The order of temporal accuracy is also the same as both ADE and PLRC methods. It is also interesting to note that the complex numerical permittivities of DE_{cor} and PE_{cor} are exactly the same although their update equations originate from different relations. Hence, PE_{cor} is an alternative reformulation of DE_{cor} which will yield the same computations but with less memory. For JE_{cor}, the transformation from frequency to Z domain is performed with an additional zero ($j\omega$) as seen from (16), which results in a different complex numerical permittivity than DE_{cor} and PE_{cor}.

Having tabulated all the relevant complex numerical permittivities, the dispersion relation of (20) is complete and it can be shown that (20) converges to the analytical dispersion relation when all the discretizations in time and space are infinitesimally small. As Δt, Δx, Δy, $\Delta z \to 0$, $\boldsymbol{K} \to \boldsymbol{k}$, $\Omega \to \omega$, $\epsilon_{nc} \to \epsilon(\omega)$ and (20) reduces to the familiar analytical dispersion relation $\boldsymbol{k}\cdot\boldsymbol{k} = \omega^2\mu_0\epsilon(\omega)$. It can also be seen that for different methods, ϵ_{nc} converges to analytical $\epsilon(\omega)$ at a different rate due to different order of the leading error term. Obviously, corrected impulse invariance method has the convergence rate twice that of classical impulse invariance method.

V. NUMERICAL RESULTS

The scalar wave numbers k_x, k_y, and k_z of (20) at each direction can be solved to obtain the dispersion characteristics of a particular method. If only 1D propagation in z-direction is considered, k_z can be expressed explicitly as

$$k_z = \frac{2}{\Delta z}\sin^{-1}\left(\frac{\Delta z\sqrt{\mu_0\epsilon_{nc}}}{\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right) \tag{21}$$

Note that k_z is complex in nature and can be compared to the analytical wave number $k(\omega) = \omega\sqrt{\mu_0\epsilon(\omega)}$. The real and (negative) imaginary parts of k are associated with the phase and attenuation constants respectively. We further define the normalized phase error as $\left|\frac{\text{Re}(k_{solved})-\text{Re}(k_{analytical})}{\text{Re}(k_{analytical})}\right|$ and normalized attenuation error as $\left|\frac{\text{Im}(k_{solved})-\text{Im}(k_{analytical})}{\text{Im}(k_{analytical})}\right|$ to facilitate the analysis.

Fig. 1(a) plots the normalized phase error and Fig. 1(b) the corresponding normalized attenuation error using various formulations for a lossy Debye medium. The Debye medium considered has three first order poles characterized by $\epsilon_s = 2046.4$, $\epsilon_\infty = 4.3$, $A_1\Delta\epsilon = 1970$, $A_2\Delta\epsilon = 30.8$, $A_3\Delta\epsilon = 41.3$, $\tau_1 = 1/(5.2\pi)\,\mu$s, $\tau_2 = 1/(680\pi)\,\mu$s, $\tau_3 = 1/(46\pi)$ns and $\sigma = 5$S/m [4]. The conductivity used here has a larger value compared to [4] so that its effect can be demonstrated clearly. The cell size Δz and time step Δt are set at 37.5μm and 0.125ps respectively. It can be seen from

TABLE III
LIST OF COMPLEX NUMERICAL PERMITTIVITY AND LEADING ERROR TERM FOR DEBYE MEDIA

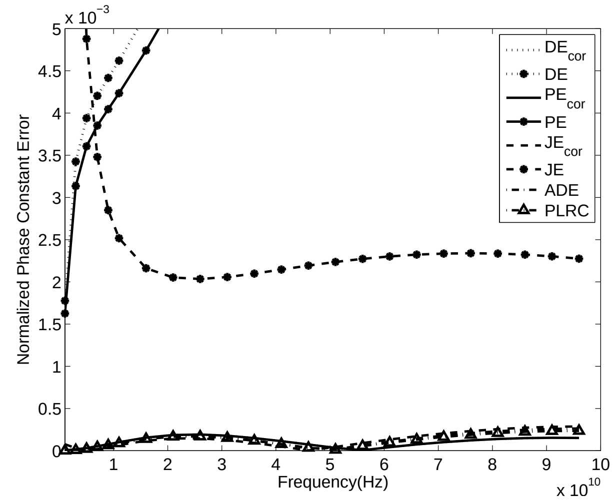
Method	Complex Numerical Permittivity	Leading Error Term
DE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{A_p\epsilon_0\Delta\epsilon\Delta t}{2\tau_p}\coth(a) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2\Big(\sum_p \frac{A_p\epsilon_0\Delta\epsilon}{12\tau_p^2}(1+j\omega\tau_p) + \frac{j\omega\sigma}{12}\Big)$
PE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{A_p\epsilon_0\Delta\epsilon\Delta t}{2\tau_p}\coth(a) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2\Big(\sum_p \frac{A_p\epsilon_0\Delta\epsilon}{12\tau_p^2}(1+j\omega\tau_p) + \frac{j\omega\sigma}{12}\Big)$
JE_{cor}	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda A_p\epsilon_0\Delta\epsilon}{j\Omega\tau_p}\Big(1 - \frac{\Delta t}{2\tau_p}\coth(a)\Big) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2\left(\sum_p \frac{A_p\epsilon_0\Delta\epsilon}{12\tau_p^3}\frac{\left(j-2\omega\tau_p - j\omega^2\tau_p^2-\omega^3\tau_p^3\right)}{\omega\left(1+j\omega\tau_p\right)} + \frac{j\omega\sigma}{12}\right)$
DE	$\epsilon_0\epsilon_\infty + \sum_p \frac{A_p\epsilon_0\Delta\epsilon\Delta t}{2\tau_p}\frac{e^a}{\sinh(a)} + \frac{\sigma e^{j\omega\Delta t/2}}{j\Omega}$	$\Delta t\Big(\sum_p \frac{A_p\epsilon_0\Delta\epsilon}{2\tau_p} + \frac{\sigma}{2}\Big)$
PE	$\epsilon_0\epsilon_\infty + \sum_p \frac{A_p\epsilon_0\Delta\epsilon\Delta t}{2\tau_p}\frac{e^a}{\sinh(a)} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t\sum_p \frac{A_p\epsilon_0\Delta\epsilon}{2\tau_p}$
JE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda A_p\epsilon_0\Delta\epsilon}{j\Omega\tau_p}\Big(1 - \frac{\Delta t}{2\tau_p}\frac{e^a}{\sinh(a)}\Big) + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t\sum_p \frac{jA_p\epsilon_0\Delta\epsilon}{2\omega\tau_p^2}$
ADE	$\epsilon_0\epsilon_\infty + \sum_p \frac{\Lambda A_p\epsilon_0\Delta\epsilon}{\Lambda + j\Omega\tau_p} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2\left(\sum_p \frac{-jA_p\epsilon_0\Delta\epsilon\omega^3\tau_p}{12\left(1+j\omega\tau_p\right)^2} + \frac{j\omega\sigma}{12}\right)$
$PLRC$ (notations can be found in [8], [9])	$\epsilon_0\epsilon_\infty + \sum_p \frac{\chi_p^0\epsilon_0 e^{j\omega\Delta t/2}}{j\Omega\Delta t} - \sum_p \epsilon_0\iota_p\chi_p^0 - \sum_p \frac{\Delta\chi_p^0\epsilon_0 e^{\frac{\Delta t}{2\tau_p}}\left(1+\iota_p\left(e^{-j\omega\Delta t}-1\right)\right)}{j2\Omega\Delta t\sinh(a)} + \frac{\sigma\Lambda}{j\Omega}$	$\Delta t^2\left(\sum_p \frac{-A_p\epsilon_0\Delta\epsilon\omega^2}{12\left(1+j\omega\tau_p\right)} + \frac{j\omega\sigma}{12}\right)$

$a = \frac{\Delta t}{2\tau_p} + \frac{j\omega\Delta t}{2}, \quad \Lambda = \cos(\omega\Delta t/2)$

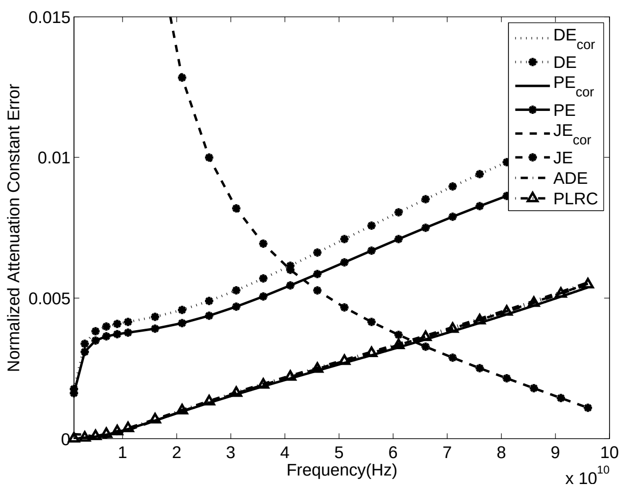
Fig. 1(a) and Fig. 1(b) that all corrected impulse invariance methods generally yield much lower normalized phase and attenuation errors than all classical impulse invariance methods, and they have approximately the same level of errors exhibited by ADE and PLRC methods. These again reaffirm the fact that corrected impulse invariance method has higher order of temporal accuracy than classical impulse invariance method. For JE, both normalized phase and attenuation errors increase dramatically as the frequency decreases. This can be understood from its leading error term where it is inversely proportionate to ω as seen from Table III.

Furthermore, we can see that DE has both higher normalized phase and attenuation errors compared to PE. By refering to Table III, it can be seen that the first order leading error term of DE involves additional conductivity term compared to PE, which further degrades the performance. As a matter of fact, although PE has first order leading error term, the error term associated to conductivity is of second order. To explain this, we can see from (13) that the conversion from frequency to Z domain of PE does not involve conductivity term. Instead, the conductivity term appears in Ampere's law (14) where central approximation and time averaging are used. On the other hand, the conversion made by DE involves the conductivity term directly as seen from (10). Therefore, invoking classical impulse invariance method will cause only the DE to have lower order of temporal accuracy for the conductivity term. For clearer illustration, let us refer to the second entry of Table I which has similar form of frequency domain transfer function as the conductivity term in (10). The transformation into Z domain using the corrected impulse invariance method is equivalent to taking the central difference approximation with time averaging at time index $n + \frac{1}{2}$. Invoking classical impulse invariance method is seen only as taking the backward difference approximation at time index $n+1$, which is of one order lower in temporal accuracy. From this, the higher order temporal accuracy of corrected impulse invariance method compared to classical impulse invariance method becomes even more intuitive and apparent.

Next, we consider 1D wave propagation in a homogeneous Debye medium of 1000 cells. The cell size Δz and time step Δt are again set at 37.5μm and 0.125ps respectively. We consider the characterization of a lossy Debye medium with one first order pole, where $\epsilon_s = 81$, $\epsilon_\infty = 1.8$, $A_1 = 1$, $\tau_1 = 47$ps and $\sigma = 0.1$S/m. Plane wave propagation is initiated by a hard source Gaussian pulse excitation at initial point. The E field in space is traced after certain time steps and the result can be compared to the analytical solution obtained by numerically integrating the exact frequency domain solution. Fig. 2(a) shows the absolute electric field error versus cell position in the Debye medium, computed using various classical impulse invariance methods after 3000 time steps. Fig. 2(b) on the other hand shows the numerical results obtained by using various corrected impulse invariance methods, as well as ADE and PLRC methods. Note the different scales used in both Y axes, which clearly indicate that all corrected impulse invariance methods achieve lower error than classical impulse invariance methods. From Fig. 2(b), it is also interesting to observe that in this case, the numerical error of JE_{cor} is the lowest among

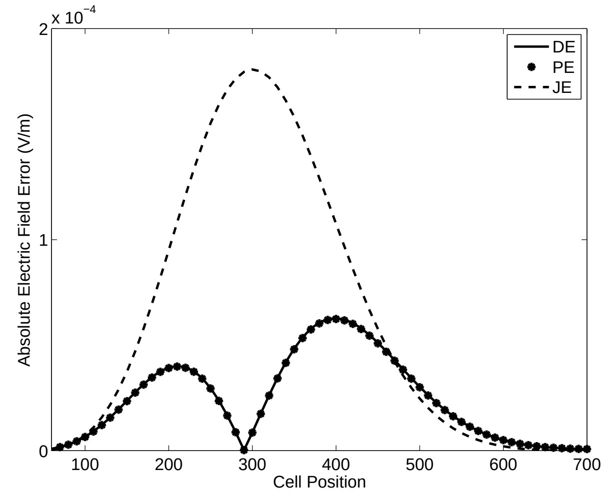


(a)

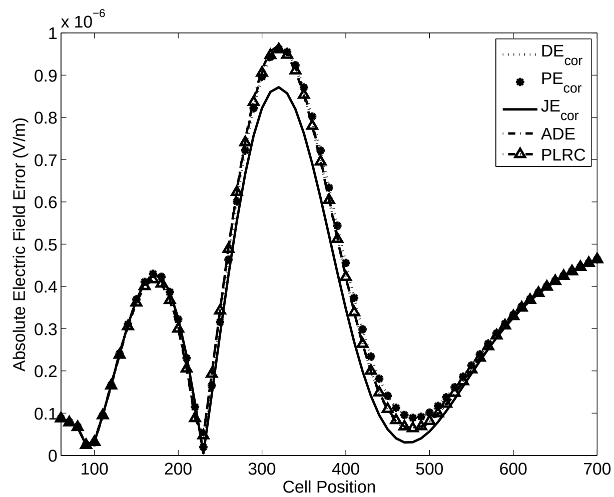


(b)

Fig. 1. Normalized (a) phase and (b) attenuation errors versus frequency using various formulations for a lossy Debye medium. All classical impulse invariance methods generally result in higher dispersion errors than corrected impulse invariance methods.



(a)



(b)

Fig. 2. Absolute electric field error versus cell position computed using various formulations of (a) classical and (b) corrected impulse invariance methods in a lossy Debye medium. All classical impulse invariance methods cause higher computed electric field error than corrected impulse invariance methods.

all, even lower than that of existing ADE and PLRC methods.

Thus far, we have considered the applications of corrected impulse invariance method in various formulation schemes for lossy Debye media. The method can be extended to other frequency-dependent media in a similar and convenient manner. As a preliminary example, Fig. 3 shows the comparison of numerical errors among corrected impulse invariance (DE_{cor}), ADE and PLRC methods in a lossy Lorentz medium. The medium is characterized by $\epsilon_s = 3$, $\epsilon_\infty = 1.5$, $A_1 = 1$, $\omega_1 = 40\pi$GHz, $\delta_1 = 0.1\omega_1$ and $\sigma = 0.1$S/m where ω_1 is the resonant frequency and δ_1 is the damping coefficient. The plot clearly indicates that DE_{cor} has the lowest numerical error among all. Again, this result reflects that the corrected impulse invariance method has the potential of achieving greater accuracy than the existing ADE and PLRC methods. This should call for further investigation and discussion on different formulation schemes of the corrected impulse invariance method in various media.

VI. Conclusion

We have presented the thorough discussions of corrected impulse invariance method in the realm of Z-transform theory for dispersive media. The correction has been shown to be necessary for dispersive media which exhibit discontinuity at $t = 0$ in the time domain susceptibility function. A (corrected) Z-transform table has been provided to facilitate the conversion from frequency to Z domain. With the aid of the table, various formulations using both corrected and classical impulse invariance methods have been carried out conveniently. Detailed performance measures such as numerical permittivity, leading error term, dispersion relation, normalized phase and attenuation errors as well as memory storage requirements have been included along with some extensive numerical comparisons.

It has been demonstrated that using certain formulation, the corrected impulse invariance method can be potentially more

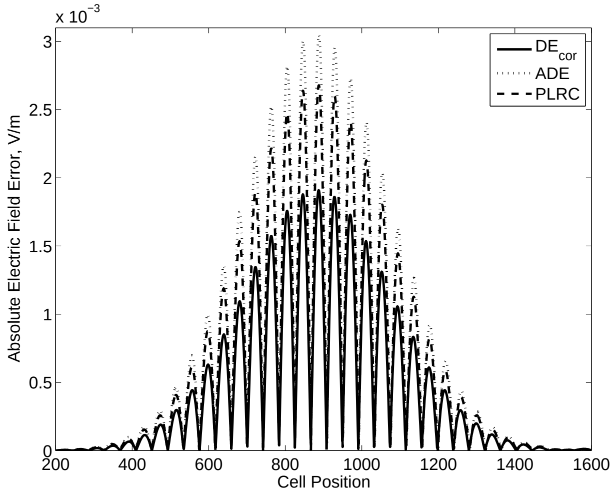


Fig. 3. Absolute electric field error versus cell position for various methods in a lossy Lorentz medium. It is observed that corrected impulse invariance method has the lowest numerical error among all.

superior compared to exisiting schemes such as ADE and PLRC methods. The effects of material parameters, temporal and spatial discretizations on the numerical errors which result from different complex numerical permittivity are beyond the scope of this paper, and can be further analyzed in the future. It is hoped that this paper has clearly pointed out the shortcomings that may be encountered by the classical impulse invariance method, and all the corrections necessary for improving the method. These corrections will be useful, not only in deriving the update equations for dispersive media, but also for all other areas, such as the development of absorbing boundary condition, perfectly matched layer (PML), etc. The corrected impulse invariance method herein may be extended as well for unconditionally stable FDTD schemes [21].

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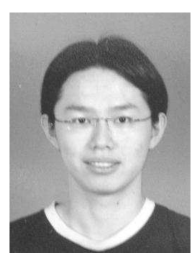

Ding Yu Heh (S’08) received the B.Eng. degree (first class honors) from Multimedia University, Cyberjaya, Malaysia, and the M.Sc. degree from Nanyang Technological University, Singapore in 2006 and 2007, respectively. He is currently working toward the Ph.D. degree in the School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore. His research areas are focused mainly on computational electromagnetics, RF and microwave circuit design.

Eng Leong Tan (SM’00) received the B.Eng. degree with first class honors from the University of Malaya, Malaysia, and the Ph.D. degree from Nanyang Technological University, Singapore. From 1991 to 1992, he was a Research Assistant at the University of Malaya. From 1991 to 1994, he worked part-time at Commercial Network Corporations Sdn. Bhd., Malaysia. From 1999 to 2002, he was a Member of Technical Staff at the Institute for Infocomm Research, Singapore. Since 2002, he has been an Assistant Professor at the School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore. His research interests include electromagnetic and acoustic simulations, RF and microwave circuit design.