

# SIMULATING POLYDISPERSE MATERIALS WITH DISTRIBUTIONS OF THE DEBYE MODEL

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**ABSTRACT.** We investigate models which approximate frequency dependent dielectric permittivity. The Cole-Cole has been shown as an excellent approximation to true data for polydisperse materials, yet time-domain simulations for this model are difficult to develop and analyze. Thus, we appeal to distributions of the Debye model represented by the method of polynomial chaos. We describe a time-stepping approach which employs Huen's method coupled with the Yee scheme. We in turn, wish to study the stability properties of our numerical scheme. We show the stability analysis for multi-pole Debye. A similar method can be applied to study the stability properties for the polynomial chaos representation.

## 1. INTRODUCTION

In electromagnetic interrogation, a pulse is sent through a dispersive dielectric material. Specifically, we are concerned with an ultra wide bandwidth (UWB) electromagnetic pulse which exhibits a range of frequencies. While Debye dispersive dielectric media such as water are well understood, problems of physical interest arise which are not well-understood. These simulations of interest are generally for polydisperse material such as the example of a dry skin sample as well as those which exhibit multiple poles (i.e. peaks in relaxation time distribution  $\tau$ ). We wish to investigate distributions of the parameter  $\tau$  for the Debye model in comparison to the heuristic Cole-Cole model which proves to be the closest approximation to experimental data.

Prior work investigated uniform distributions of  $\tau$  in the Debye model, but we hope to extend this further. Specifically, the literature ascertains that the log-normal distribution of Debye reasonably approximates the distribution corresponding to the Cole-Cole model for some values of distribution parameter  $\alpha$ . Ultimately, it is hoped to simulate an electromagnetic pulse in the time domain for polydispersive materials, and since the Cole-Cole model proves difficult in such simulations, we appeal to distributions of Debye instead. From here we proceed in the simulation of an ordinary differential equation while exploring various numerical methods. Finally, for such a numerical method, one must verify the stability. For our purposes, we consider second-order accurate methods for a representation of the multi-pole Debye model with the end goal in mind to verify the stability for the polynomial chaos method.

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## 2. BACKGROUND

**2.1. Maxwell's Equations.** First we introduce Maxwell's equations which govern the behavior of electromagnetic fields and are what we wish to simulate in a dispersive dielectric media, namely a Debye dispersive media. The following gives the differential form of Maxwell's equations in terms of free current and free charge such that  $\mathbf{E}$  and  $\mathbf{H}$  are electric and magnetic fields, respectively,  $\mathbf{D}$  and  $\mathbf{B}$  are electric and magnetic flux densities, respectively, and scalar  $\rho$  represents the density of free electric charges unaccounted for in the electric polarization. The conduction current density is given by  $\mathbf{J}$ .

$$(1) \quad \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H}$$

$$(2) \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$(3) \quad \nabla \cdot \mathbf{D} = \rho$$

$$(4) \quad \nabla \cdot \mathbf{B} = 0.$$

Also important to note are the constitutive laws which complete Maxwell's equations by describing the response of the medium to the electromagnetic field.

$$(5) \quad \mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

$$(6) \quad \mathbf{B} = \mu \mathbf{H} + \mathbf{M}$$

$$(7) \quad \mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_s,$$

Additionally defined vectors include polarization  $\mathbf{P}$ , magnetization  $\mathbf{M}$ , and source current density  $\mathbf{J}_s$ . Additionally defined scalars include permittivity  $\epsilon$  such that  $\epsilon = \epsilon_0 \epsilon_\infty$  (with  $\epsilon_0$  the permittivity of free space and  $\epsilon_\infty$  the infinite frequency electric permittivity), the magnetic permeability  $\mu$ , and the electric conductivity  $\sigma$ .

We combine Maxwell's equations with the constitutive laws for the purpose of simulation. Through the use of appropriate initial conditions and boundary conditions, substitution of the constitutive laws into Maxwell's curl equations yields the following equations. Also, for simplification, we assume no magnetization.

$$(8) \quad \epsilon \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J} - \frac{\partial \mathbf{P}}{\partial t} = \nabla \times \mathbf{H} - \sigma \mathbf{E} - \mathbf{J}_s - \frac{\partial \mathbf{P}}{\partial t}.$$

$$(9) \quad \mu \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}.$$

We wish to simplify our problem to one spacial dimension. Assume that the electric field oscillates in the  $xz$ -plane and travels in the  $z$ -direction. Now recall that since electromagnetic waves are transverse, their oscillation is perpendicular to the  $z$ -direction of propagation, and hence  $E_z$  and  $H_z$  equal zero. Thus, this simplification results in the following equations.

$$(10) \quad \epsilon \frac{\partial E_x}{\partial t} = -\frac{\partial H_y}{\partial z} - \sigma E_x - \frac{\partial P_x}{\partial t} - J_s.$$

$$(11) \quad \mu \frac{\partial H_y}{\partial t} = -\frac{\partial E_x}{\partial z}.$$

**2.2. Dispersive Media.** For our purposes we are concerned with Maxwell's equations in Debye media which is a dispersive dielectric media. Note that the dispersiveness of such a media refers to the media's permittivity depending on angular frequency  $\omega$  of the waves which pass through it (recall  $\omega = 2\pi f$  where  $f$  is frequency in Hz), and dielectric simply means that the material is non-conductive. Recall from the constitutive laws the polarization vector  $\mathbf{P}$ . The polarization expresses the density of the electric dipole moments in the dielectric. Contained in the polarization are the dielectric parameters of interest;  $\epsilon_\infty$ , the infinite frequency permittivity;  $\epsilon_s$ , the static permittivity which is the permittivity at the limit of zero frequency and;  $\tau$ , the dipolar relaxation time of the medium. We are interested in further exploration of the dielectric parameter  $\tau$ , especially for poly-disperse material (i.e. those which exhibit a distribution of relaxation times) which are of physical interest.

**2.3. Dielectric Response Functions.** Consider a function  $g(t, \mathbf{x})$  known as a dielectric response function (DRF). This function characterizes the dielectric material and can be thought of as the "memory" effect of the dielectric. Now we write polarization as a convolution of the DRF and the applied electric field which gives

$$(12) \quad \mathbf{P}(t, \mathbf{x}) = g \star \mathbf{E}(t, \mathbf{x}) = \int_0^t g(t-s, \mathbf{x}; \mathbf{v}) \mathbf{E}(s, \mathbf{x}) ds$$

with  $\mathbf{v} = \{\epsilon_s, \epsilon_\infty, \tau\}$ .

$$(13) \quad \tau \dot{\mathbf{P}} + \mathbf{P} = \epsilon_d \mathbf{E}$$

Now for the Debye model of dipolar relaxation for dispersive media, the DRF is given by

$$(14) \quad g(t, \mathbf{x}) = \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau} e^{-t/\tau}.$$

The polarization above can be shown to be equivalent to the solution of the ordinary differential equation, with  $\epsilon_d = \epsilon_0(\epsilon_s - \epsilon_\infty)$ . A heuristic generalization of the Debye model is the Cole-Cole model whose DRF is given by,

$$(15) \quad g(t, \mathbf{x}) = \frac{1}{2\pi i} \int_{\zeta-i\infty}^{\zeta+i\infty} \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{1 + (s\tau)^{1-\alpha}} e^{st} ds.$$

**2.4. Complex Dielectric Permittivity.** Consider dielectric permittivity  $\epsilon$  as a function of angular frequency  $\omega$ . It can be shown that  $\epsilon(\omega)$  can be expressed as the Fourier transform of the dielectric response function  $g(t)$  in the time domain which gives,

$$(16) \quad \epsilon(\omega) = \epsilon'(\omega) - i\epsilon''(\omega) = \epsilon_\infty + \int_0^\infty g(t) e^{-i\omega t} dt.$$

To understand this function physically, we appeal to losses in alternating current capacitors. Conduction loss in an ac capacitor refers to the flow of actual charge through the dielectric while the dielectric loss occurs from the movement or rotation of atoms or molecules in the alternating electric field. In the above equation, the real part of the permittivity  $\epsilon' = \epsilon_r \epsilon_0$  represents the ac capacity, which can be thought of as the stored energy, where  $\epsilon_r$  is the dielectric constant of the medium. The imaginary part of the permittivity  $\epsilon''$  represents the dielectric loss factor, or stored

losses in the medium, and additionally we get the ratio  $\tan \delta = \frac{\epsilon''}{\epsilon'}$  which is called the loss tangent or dissipation factor. In classical Debye theory, the difference between  $\epsilon_0$  and  $\epsilon_\infty$  is due to dipolar polarization. The orientation of polar molecules in an alternating-current field is opposed by the effects of thermal agitation and molecular interactions [7].

We can demonstrate how complex permittivity  $\epsilon(\omega)$  relates to our previous discussion by converting the constitutive law  $\mathbf{D} = \epsilon_\infty \mathbf{E} + \mathbf{P}$  to the frequency domain. Recall that polarization is defined as a convolution so since  $\mathbf{P} = g \star \mathbf{E}(t, \mathbf{x})$  thus  $\hat{\mathbf{P}} = \hat{g} \hat{\mathbf{E}}$  where  $\hat{\mathbf{P}}$ ,  $\hat{g}$  and  $\hat{\mathbf{E}}$  are the Fourier transforms of polarization, the DRF, and the electric field respectively. Given transformed polarization

$$(17) \quad \hat{\mathbf{D}} = \epsilon_\infty \hat{\mathbf{E}} + \hat{\mathbf{P}}$$

then becomes

$$(18) \quad \hat{\mathbf{D}} = (\epsilon_\infty + \hat{g}) \hat{\mathbf{E}}$$

This then gives us the following relation between electric field and electric flux density in a Debye medium such that  $\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 - i\omega\tau}$ ,

$$(19) \quad \hat{\mathbf{D}} = \epsilon(\omega) \hat{\mathbf{E}}.$$

**2.5. Debye and Cole-Cole Models.** For a Debye medium, the complex dielectric constant as a function of frequency has the following expression for multiple poles,

$$(20) \quad \epsilon(\omega)_D = \epsilon_\infty + \sum_{m=1}^n \frac{\Delta\epsilon_m}{1 + (i\omega\tau_m)} + \frac{\sigma}{i\omega\epsilon_0}.$$

Other empirical models exist such as the Cole-Cole, the Davidson-Cole, and the Havriliak-Negami which attempt to approximate  $\epsilon(\omega)$  [4]. The Cole-Cole model is given by,

$$(21) \quad \epsilon(\omega)_{CC} = \epsilon_\infty + \sum_{m=1}^n \frac{\Delta\epsilon_m}{1 + (i\omega\tau_m)^{(1-\alpha_m)}} + \frac{\sigma}{i\omega\epsilon_0}.$$

In both of these models,  $\tau_m$  represents the relaxation time parameter and we have  $\Delta\epsilon_m = \epsilon_{sm} - \epsilon_{sm-1}$  with  $\Delta\epsilon_1 = \epsilon_{s1} - \epsilon_\infty$ . The distribution of relaxation times in this model are characterized by the parameter  $0 \leq \alpha \leq 1$ .

### 3. LITERATURE SEARCH MOTIVATION

Work from the past summer has shown that using a uniform distribution of the relaxation time dielectric parameter  $\tau$  improved the Debye model in terms of fit to true data for a dispersive dielectric media, but this model never provided a closer approximation than the Cole-Cole model which is a function to approximate the frequency response of polydisperse materials. However, physically, the relaxation times vary among molecules which suggests that a log-normal distribution of  $\tau$  is more appropriate. We wished to investigate transformations of functions with distributions of parameters as well as numerical simulations for distributions of Debye. Generally, we wished to gain a better understanding of previous research relating to the Cole-Cole model and distributions of Debye in order to develop a meaningful and worthwhile project.

Support for the notion of distributions of relaxation times was first motivated by von Schweidler's work where upon the investigation of the mechanisms of absorption in dielectrics, equations

for frequency variations of  $\epsilon'$  and  $\epsilon''$  proved inadequate in describing experimental results even though mechanisms of dielectric absorption indicate a simple exponential function. It is generally agreed that these discrepancies between experiment and theory are to be attributed to the poly-disperse nature of materials [25]. Yager investigates a method for obtaining agreement between experimental data on dispersion and dielectric loss as well as agreement between the theoretical and experimental curves for frequency variation of  $\epsilon'$  and  $\epsilon''$ . Note that the experimental distributions are calculated by the "circular arc locus" plots of  $\epsilon'$  versus  $\epsilon''$  [7]. Yager notes that von Schweidler's extension "assumes a large number of different kinds of particles having different relaxation times." He notes that the relaxation function can be written in such a way to sum the different relaxation times,

$$(22) \quad \Phi(t) = \sum_1^n \frac{k_n e^{-\frac{t}{\tau_n}}}{\tau_n}$$

where  $k_n$  is proportional to the number of particles per unit volume and  $\tau_n$  represents relaxation time. As the number  $n$  approaches infinity, the relaxation times vary continuously from 0 to  $\infty$ , so we can substitute the integral,

$$(23) \quad \Phi(t) = \int_0^\infty \frac{k_n e^{-\frac{t}{\tau}}}{\tau} d\tau$$

with  $k_t$  representing the distribution of relaxation times. This formulation presents an appropriate distribution function which can be generally extended to relaxation functions. By substitution into the "reversible absorption current" function, we get the following formulas for the real and complex parts of permittivity, respectively.

$$(24) \quad \epsilon' = \epsilon_\infty \left[ 1 + \int_0^\infty \frac{k(\tau)}{1 + \omega^2 \tau^2} d\tau \right]$$

$$(25) \quad \epsilon'' = \epsilon_\infty \int_0^\infty \frac{k(\tau) \omega \tau}{1 + \omega^2 \tau^2} d\tau$$

Similar derivations of such equations are also described in Fuoss and Kirkwood [8] where function  $G(\tau)$  is given as the distribution function and  $G(\tau)d\tau$  specifies the fraction of total dipole moment of a molecule associated with relaxation times in the interval between  $\tau$  and  $\tau + d\tau$ . Also note for such a condition that the distribution function must also meet a normalization condition of the total dielectric strength which is given by  $\int_0^\infty G(\tau)d\tau = 1$ . Wagner proposed that this general distribution function of relaxation times is governed by the probability function known as the log-normal distribution which is given by

$$(26) \quad k(\tau)d\tau = \frac{kb}{\pi^{1/2}} e^{-b^2 z^2} dz$$

with  $z = \ln \frac{\tau}{\tau_0}$  and the density or breadth of the distribution determined by the constant  $b$ . To make sense of this formula, note that it simply states that the logarithms of the relaxation times are grouped about the logarithm of the most prominent relaxation time  $\tau_0$  [25]. Discussion of a similar nature is abundant in [4], [7], [12], and [19].

However, the log-normal is not the only appropriate distribution to consider. We see that the Cole-Cole and other heuristic models have a corresponding distribution function we will call  $G(\tau)$

which describes "the superposition of exponentially damped processes" [4]. Corresponding to the Cole-Cole model, we have the distribution,

$$(27) \quad G(\tau) = \frac{1}{2\pi} \left[ \frac{\sin(\alpha\pi)}{\cosh(\alpha \ln(\tau/\tau_0)) - \cos(\alpha\pi)} \right].$$

where  $\alpha$  is calculated from the circular arc locus of the Cole-Cole plot [19]. Moreover, we see that given any empirical formula for  $\epsilon(\omega)$ , one can analytically calculate the expression for  $G(\tau)$  by applying the inverse Stieltjes transform to the equation for  $\epsilon(\omega)$ . This transform is given by [4] as follows,

$$(28) \quad G(\tau) = \frac{1}{2\pi i} \left[ \epsilon \left( \frac{e^{-i\pi}}{\tau} \right) - \epsilon \left( \frac{e^{i\pi}}{\tau} \right) \right].$$

Motivation behind the log-normal distribution of the relaxation times in the Debye model representing an appropriate approximation for polydisperse materials lies with a comparison of the log-normal distribution to the distribution corresponding to the Cole-Cole model. Also, as suggested in [1], an efficient way of making a connection between the parameters of the models without resorting to Fourier transforms can be done by computing the distributions corresponding to time domain polarization models and comparing them to distributions corresponding to frequency domain polarization models. Concentrating solely on the corresponding distribution to the log-normal and  $G(\tau)$ , we see that plots of the aforementioned distributions most closely match when  $b = 0.6$  and  $\alpha = 0.23$ . As the value of  $\alpha$  increases beyond this point, the log-normal distribution becomes a poorer approximation [7]. However, the reasonable closeness of the functions at lower values of  $\alpha$  warrants further investigation into a log-normal distribution of relaxation times for a time domain simulation of polydisperse materials. Although this distribution presents itself as the ideal one because of its closeness to distribution  $G(\tau)$  while presenting a greater ease to work with, it is important to keep in mind that many experimentalists have used an approach of the uniform distribution, which we call  $g(\tau)$  as an acceptable one. In [12], the authors cite reasons for appealing to this distribution as the "uniform  $g(\tau)$  is the simplest case and allows us to estimate the width, upper and lower limits of relaxation time distribution," such a distribution suits the dielectric spectra of PLZT and that "parameters of the uniform distribution can be easily defined from the Cole-Cole equation parameters because both uniform  $g(\tau)$  and Cole-Cole equation correspond to a symmetrical distribution of relaxation times in the logarithmic scale." In the case of the uniform distribution, our previously mentioned expressions for the real and complex parts of dielectric permittivity become the following,

$$(29) \quad \epsilon'(\omega) = \epsilon_\infty + \frac{B}{2} \ln \left( \frac{a^2 + \omega^2 \tau_1^2}{1 + \omega^2 \tau_1^2} \right)$$

and

$$(30) \quad \epsilon''(\omega) = B \tan^{-1} \left[ \frac{\omega \tau_1 (a - 1)}{\omega^2 \tau_1^2 + a} \right]$$

where we have some upper and lower limits of Debye relaxations,  $\tau_1$  and  $\tau_2$  respectively, and  $B = \frac{\Delta\epsilon}{\ln a}$  such that  $\Delta\epsilon$  is the distribution function normalized by the total dielectric strength. Additionally, we have parameter  $a = \frac{\tau_1}{\tau_2}$ . Finally, as suggested by [6] and [18], determination of

relaxation time distribution (RTD) is useful in the sciences. Specifically, it is suggested that a RTD approach is attractive due the nature of natural materials which are largely heterogeneous containing different chemical compositions and textural elements which produce multiple relaxation times. One example important in hydrogeophysics and petrophysics where determining the RDT is useful in estimating the diffusion coefficient of soil with known grain sizes. Furthermore, [6] mentions how the analysis of existing theories of polarization of heterogeneous media shows that electrical spectroscopy can be useful for the interpretation of frequency spectra of complex dielectric permittivity or conductivity of water-bearing rocks and porous materials in general and additionally can be useful in determining water content.

#### 4. DISCRETIZATION

Consider the polarization form of the equations for Debye media.

$$(31) \quad \begin{aligned} \frac{\partial H}{\partial t} &= -\frac{1}{\mu} \frac{\partial E}{\partial z} \\ \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} + \frac{\partial P}{\partial t} &= -\frac{\partial H}{\partial z} \\ P + \tau \frac{\partial P}{\partial t} &= (\epsilon_s \epsilon_0 - \epsilon_\infty \epsilon_0) E. \end{aligned}$$

We discretize these equations according to the Yee scheme using a central difference approximation for a Debye medium with two poles, which gives the following equations where  $n$  represents the time step and  $j$  represents our spatial step. The expression for the magnetic field update is given by,

$$(32) \quad H_{j+\frac{1}{2}}^{n+1} = -\frac{\Delta t}{\mu \Delta z} \left[ E_{j+1}^{n+\frac{1}{2}} - E_j^{n+\frac{1}{2}} \right] + H_{j+\frac{1}{2}}^n.$$

The approximation for the electric field update is given by,

$$(33) \quad \begin{aligned} E_j^{n+\frac{1}{2}} &= \frac{\theta}{1+\delta} \left( H_{j+\frac{1}{2}}^n - H_{j-\frac{1}{2}}^n \right) + \frac{1-\delta}{1+\delta} E_j^{n-\frac{1}{2}} \\ &+ \frac{2\Delta t}{\epsilon(2\tau_1 + \Delta t)(1+\delta)} P_{j,1}^{n-\frac{1}{2}} + \frac{2\Delta t}{\epsilon(2\tau_2 + \Delta t)(1+\delta)} P_{j,2}^{n-\frac{1}{2}}, \end{aligned}$$

where  $\theta = -\frac{\Delta t}{\epsilon \Delta z}$  and the loss term is defined as  $\delta = \frac{\Delta t \epsilon_{d1}}{\epsilon_\infty(2\tau_1 + \Delta t)} + \frac{\Delta t \epsilon_{d2}}{\epsilon_\infty(2\tau_2 + \Delta t)}$ . Note here that we are assuming that conductivity  $\sigma = 0$ . In (33) we see that the electric field update is dependent on both polarization expressions which are given by,

$$(34) \quad P_{j,1}^{n+\frac{1}{2}} = \frac{\Delta t \epsilon_0 \epsilon_{d1} \left[ E_j^{n+\frac{1}{2}} + E_j^{n-\frac{1}{2}} \right] + (2\tau_1 - \Delta t) P_{j,1}^{n-\frac{1}{2}}}{2\tau_1 + \Delta t},$$

and similarly,

$$(35) \quad P_{j,2}^{n+\frac{1}{2}} = \frac{\Delta t \epsilon_0 \epsilon_d 2 \left[ E_j^{n+\frac{1}{2}} + E_j^{n-\frac{1}{2}} \right] + (2\tau_2 - \Delta t) P_{j,2}^{n-\frac{1}{2}}}{2\tau_2 + \Delta t}.$$

## 5. POLYNOMIAL CHAOS

Sets of orthogonal polynomials can be used to approximate any continuous function, and if infinitely many are used, to give the exact function. When working with parameters that are represented by a distribution, that parameter, which is called a random variable can be represented by a series of polynomials. Transforming the distribution in a set of polynomials is advantageous because polynomials are easy to both integrate and differentiate, and having orthogonal ones allows us to distinguish between them easily.

In taking a finite number of polynomials to approximate our distribution, convergence is an important issue. The best polynomials are given in [13] to use various distributions, including Gaussian and Uniform, unfortunately we could neither find nor derive an efficient way of approximating our theorized Lognormal distribution for  $\tau$ , so we used this method to approximate a uniform distribution of  $\tau$ .

We begin by assuming that the function,  $x$ , of the distribution of our random variable,  $\xi$ , can be represented by a set of finite polynomials, since we are doing a uniform distribution, we will use Legendre polynomials [13]. In this section we use the notation from Lucor's paper. This gives us

$$(36) \quad x(t, \xi) = \sum_{j=0}^p \alpha_j(t) P_j(\xi).$$

We will use this set of polynomials to solve the differential equation  $k(\xi) \dot{i}(\xi) = -t(\xi) + E(\xi)$ . We set  $k = \sigma r + \gamma$ . To simplify the left hand side we use the recursion relations for Legendre polynomials

$$(37) \quad \xi P_j(\xi) = \frac{j+1}{2j+1} P_{j+1}(\xi) + \frac{j}{2j+1} P_{j-1}(\xi).$$

Substituting this into our differential equation, we get

$$(38) \quad \sum_{j=0}^p \dot{\alpha}_j \left( \sigma \frac{j+1}{2j+1} P_{j+1}(\xi) + \sigma \frac{j}{2j+1} P_{j-1}(\xi) \right) + \gamma P_j = E - \sum_{j=1}^p \alpha_j.$$

We now take the inner product of this with respect to the Legendre polynomials, this gives, for  $j = 0$ ,

$$(39) \quad 2 \left( \gamma \dot{\alpha}_0 + \frac{1}{3} \sigma \dot{\alpha}_1 + \alpha_0 \right) = \epsilon_0 \epsilon_D E$$

And for all other  $j$ ,

$$(40) \quad \gamma \dot{\alpha}_j + \sigma \frac{j}{2j-1} \dot{\alpha}_{j-1} + \sigma \frac{j+1}{2j+1} \dot{\alpha}_{j+1} + \alpha_j = 0$$



These coupled differential equations can be combined in a matrix equation and solved using the Improved Euler Method. We use the expected value of the polarization to force the electric field.

## 6. STABILITY ANALYSIS

As previously mentioned, we are interested in broadband interrogation and time domain simulations of polydisperse materials, such as dry skin, which have multiple poles (i.e. peaks in the distribution) which are not Debye. In order to model such materials, we must either appeal to the Cole-Cole model or the Debye model with distributions of relaxation times. However, one must determine the stability of the numerical method as in [10] and [3]. One might wonder the significance of stability. In general, we wish for our numerical scheme to better approximate Maxwell's equations as the spatial and temporal step sizes are reduced. Such a scheme is known as convergent. The term consistency means that our discretized version of the partial differential equations in question only differs by factors which go to zero as  $\Delta$  and  $\Delta t$  also go to zero [10]. The following theorem, known as the Lax-Richtmyer Equivalence Relation, combines the ideas of stability, consistency, and convergence.

**Theorem 6.1.** *A consistent finite difference scheme for a partial differential equation for which the initial value problem is well-posed is convergent if and only if it is stable.*

Ultimately, we wish to compare the stability analysis for simulating electric fields having distributions of relaxation times with a previous stability analysis for Cole-Cole. We start by considering the stability analysis for the discretization of the equations for the Debye media in polarization form. Now, plane wave solutions of (32), (33), (34), and (35) are of the form,

$$(41) \quad \begin{bmatrix} H_j^n \\ E_j^n \\ P_{j,1}^n \\ P_{j,2}^n \end{bmatrix} = \begin{bmatrix} \tilde{h} \\ \tilde{e} \\ \tilde{p}_1 \\ \tilde{p}_2 \end{bmatrix} \zeta^n e^{ikj\Delta z}.$$

Here,  $k = \frac{\omega}{c}$  represents the wave number with  $c$  the speed of light and  $\vec{x} = [\tilde{h}; \tilde{e}; \tilde{p}_1; \tilde{p}_2]^T$  is the eigenvector corresponding to the complex time eigenvalue  $\zeta$ . Notice that the time component here is separated from the spatial component. Thus, we are separating the amplification over time to see if it blows up. To ensure stability of the method, we require that all  $\zeta$  satisfy  $|\zeta| < 1$ . Now we substitute each component of (41) into the corresponding discretized update equations which results in the following expressions,

$$(42) \quad \tilde{h}(\zeta - 1) + \left[ \frac{2\Delta t i}{\mu\Delta z} \sin\left(\frac{k\Delta z}{2}\zeta^{\frac{1}{2}}\right) \right] \tilde{e} = 0$$

$$(43) \quad \left[ (2\tau_1 + \Delta t)\zeta^{\frac{1}{2}} - (2\tau_1 + \Delta t)\zeta^{-\frac{1}{2}} \right] \tilde{p}_1 - \Delta t \epsilon_0 \epsilon_{d1} (\zeta^{\frac{1}{2}} - \zeta^{-\frac{1}{2}}) \tilde{e} = 0,$$

and similarly,

$$(44) \quad \left[ (2\tau_2 + \Delta t)\zeta^{\frac{1}{2}} - (2\tau_2 + \Delta t)\zeta^{-\frac{1}{2}} \right] \tilde{p}_2 - \Delta t \epsilon_0 \epsilon_{d2} (\zeta^{\frac{1}{2}} - \zeta^{-\frac{1}{2}}) \tilde{e} = 0,$$

and lastly,

$$(45) \quad \left( \zeta^{\frac{1}{2}} - \frac{1-\delta}{1+\delta} \zeta^{-\frac{1}{2}} \right) \tilde{e} + \left[ \frac{2\theta i}{1+\delta} \sin\left(\frac{k\Delta z}{2}\right) \right] \tilde{h} - \frac{2\Delta t}{\varepsilon(2\tau_1 + \Delta t)(1+\delta)} \zeta^{-\frac{1}{2}} \tilde{p}_1 - \frac{2\Delta t}{\varepsilon(2\tau_2 + \Delta t)(1+\delta)} \zeta^{-\frac{1}{2}} \tilde{p}_2 = 0.$$

Thus, we have the system  $A \vec{x} = \vec{0}$ , and letting  $\rho = \sin\left(\frac{k\Delta z}{2}\right)$  where

$$(46) \quad A = \begin{bmatrix} \zeta - 1 & \frac{2\Delta t i}{\mu\Delta z} \rho \zeta^{\frac{1}{2}} & 0 & 0 \\ \frac{2\theta i}{1+\delta} \rho & \zeta^{\frac{1}{2}} - \frac{1-\delta}{1+\delta} \zeta^{-\frac{1}{2}} & -\frac{2\Delta t}{\varepsilon(2\tau_1 + \Delta t)(1+\delta)} \zeta^{-\frac{1}{2}} & -\frac{2\Delta t}{\varepsilon(2\tau_2 + \Delta t)(1+\delta)} \zeta^{-\frac{1}{2}} \\ 0 & \Delta t \varepsilon_0 \varepsilon_{d1} (\zeta^{\frac{1}{2}} - \zeta^{-\frac{1}{2}}) & (2\tau_1 + \Delta t) \zeta^{\frac{1}{2}} - (2\tau_1 - \Delta t) \zeta^{-\frac{1}{2}} & 0 \\ 0 & \Delta t \varepsilon_0 \varepsilon_{d2} (\zeta^{\frac{1}{2}} - \zeta^{-\frac{1}{2}}) & 0 & (2\tau_1 + \Delta t) \zeta^{\frac{1}{2}} - (2\tau_1 - \Delta t) \zeta^{-\frac{1}{2}} \end{bmatrix}.$$

Calculating the determinant of  $A$  and setting equal to zero yields the following fourth order stability polynomial,

$$(47) \quad P = \lambda_1 \zeta^4 + \lambda_2 \zeta^3 + \lambda_3 \zeta^2 + \lambda_4 \zeta + \lambda_5,$$

Note that the discretizations for the electric field and polarization is easily generalized for any number of poles for a Debye medium. The generalized matrix of  $A$  is straightforward. The stability analysis can be completed by using MAPLE to plot  $\zeta = \max |\chi|$  where  $\chi$  are the roots of the stability polynomial. Note that we plot the maximum since the system will behave according to this eigenvalue. If the eigenvalue is greater than one this indicates that the numerical method is unstable. Also note that since we are interested in broadband electromagnetic interrogation, we must check the stability of the given scheme at different frequencies. An example of such plots for a second order accurate Debye scheme follow.

**6.1. Stability Analysis Results for Two Pole Debye.** The following plots display the stability analysis done in MAPLE for the two pole debye stability polynomial. Notice that the  $x$ -axis here is given by  $k\Delta z$  where  $k$  is the wave number as before. Thus, the meaning of such a plot has two separate interpretations. One, for fixed discretization,  $k$  will vary (but really think of frequency varying). In this case, the plot tells you which frequencies (since a UWB pulse is used) have the least dissipation error. Secondly, in the case of a fixed frequency, one can think of the discretization varying, and thus small values of  $k\Delta z$  represent really small values of  $\Delta z$  when  $k$  is fixed. Hence, if the curves are flat there really is no benefit with respect to reducing error by decreasing your discretization step. Also, note that  $k\Delta z = \frac{2*\pi}{Nppw}$  where  $Nppw$  represents the "number of points per wavelength." For example to illustrate, if  $k\Delta z = \pi$ , then  $Nppw = 2$ , which is not very refined. However, if  $k\Delta z = .5$ , then  $Nppw = 4 * \pi$  or roughly 10, which is pretty much the least one should be doing. Then, when evaluating what these curves signify, one really should pay most attention to what is happening to the left of .5. As a final note, it is evident from the plots that this method is stable as the eigenvalue is always less than one. Notice, however, that as we refine the timestep, the plot values become closer to one.

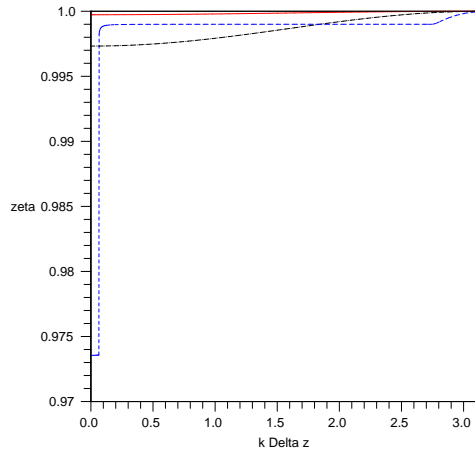


FIGURE 1. P2 with large  $\Delta t$  ;  $\nu = 1$ . The following are the given values of  $\Delta t$ : solid red,  $3.2481e - 09$ ; dashed black,  $3.241e - 10$ ; dashed blue,  $3.241e - 11$ .

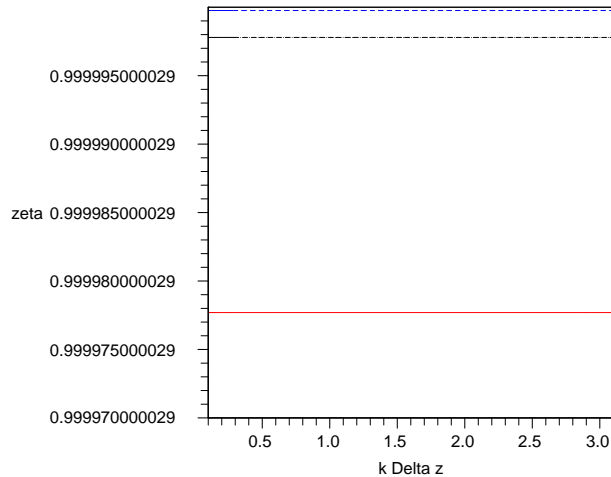


FIGURE 2. P2 with small  $\Delta t$  ;  $\nu = 1$ . The following are the given values of  $\Delta t$ : solid red,  $7.234e - 13$ ; dashed black,  $7.234e - 14$ ; dashed blue,  $7.234e - 15$ .

## 7. CONCLUSIONS AND FUTURE DIRECTIONS

We have investigated numerical methods for distributions of relaxation times in the Debye model, and we have also studied the stability analysis for multipole Debye. An extension of the stability analysis for the polynomial chaos representation has begun to be investigated; however, the next step in this process would be obtaining the correct discretized versions of the coupled equations where polarization is represented by  $\alpha_0$  and  $\alpha_1$  is the auxiliary variable. From this point, one can make the plane wave substitutions into these equations similarly to the process used for the two pole Debye stability analysis which should yield a matrix and stability polynomial.

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