Incorporating the Havriliak–Negami dielectric model in the FD-TD method
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ABSTRACT

We derive and analyze an efficient algorithm to incorporate the anomalously dispersive Havriliak–Negami dielectric model of induced polarization in the Finite-difference time-domain (FD-TD) method. Our algorithm implements this dielectric model, which in the time-domain involves fractional derivatives and fractional differential operators, with a preset error over the desired computational time interval \([0, T_{\text{comp}}]\) and correctly takes into account the singularity at \(t = 0^+\) of the corresponding time-domain dielectric susceptibility. The overall algorithm is shown to be second-order accurate in space and time, and to obey the standard FD-TD stability condition. Numerical experiments confirm our analysis.

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1. Introduction

All of the anomalously dispersive dielectric models typically employed to fit experimentally determined frequency-dependent permittivity data are subclasses of the 5-parameter Havriliak–Negami (H–N) dielectric model [1] for which the complex permittivity function takes the form

\[
\varepsilon(\omega) = \varepsilon_0 \varepsilon_\infty + \varepsilon_0 \frac{\varepsilon_\infty - \varepsilon_0}{1 + (i\omega\tau)^\alpha},
\]

where \(0 < \alpha, \beta \leq 1\), \(\tau\) is the central relaxation time of the material model, \(\varepsilon_0\) is the permittivity of vacuum, and the relative permittivities \(\varepsilon_\infty\) and \(\varepsilon_\alpha\) satisfy \(\varepsilon_\alpha > \varepsilon_\infty \geq 1\). The Debye model [2] is obtained by setting \(\alpha = \beta = 1\), while the Cole–Cole (C–C) [3] and Cole–Davidson (C–D) [4] models are obtained by setting \(\beta = 1\) and \(\alpha = 1\), respectively. The H–N dielectric model is the most general material model that arises from considerations [5] of the multi-scale nature of the spatial microstructure of a broad class of dielectrics of technological and medical interest. Typical materials whose dielectric permittivity has been represented by the H–N model include glassy materials [6], amorphous polymers near the glass-liquid transition [7], soils [8], and biological tissues [9].

Dielectric models of permittivity are typically implemented in the FD-TD [10] method by using in Ampere’s Law, \(D = \nabla \times H\), the constitutive relation \(\mathbf{D} = \varepsilon_0 \varepsilon_\alpha \varepsilon_\infty \mathbf{E} + \mathbf{P}\), where \(\mathbf{E}\) and \(\mathbf{P}\) are respectively the electric and induced polarization fields. In the case \(0 < \alpha \leq 1\), \(\beta = 1\), one approach is to determine \(\mathbf{P}\) through an auxiliary fractional differential equation that is forced by the electric field, \(\mathbf{E}\), i.e., \(\tau^\alpha D_\alpha^\beta \mathbf{P} + \mathbf{P} = \varepsilon_0 (\varepsilon_\alpha - \varepsilon_\infty) \mathbf{E}\), where \(D_\alpha^\beta\) is the fractional time derivative of order \(\alpha\), and previous works have done so for the Debye \((\alpha = 1) [11]\) and Cole–Cole \((0 < \alpha < 1) [12]\) dielectric models. In the case of the H–N model, \(0 < \alpha, \beta < 1\), this fractional differential equation is formally a fractional pseudo-differential equation \((\tau^\alpha D_\alpha^\beta + 1)\mathbf{P} = \varepsilon_0 (\varepsilon_\alpha - \varepsilon_\infty) \mathbf{E}\), which cannot be incorporated into the FD-TD method in a straightforward manner. An alternative approach, which we adopt here as described in Section 2, is to incorporate the H–N dielectric model into Ampere’s Law.
by determining $P$ in the constitutive relation via a convolution in time of the electric field with the inverse transform of the second term in (1) which represents the time-domain susceptibility, $\chi(t)$. A straightforward implementation of this convolution is computationally prohibitive due to the non-exponential nature of the kernel, $\chi(t)$, which is singular at $t = 0^+$ and decays algebraically for $t > 0^+$. The present paper offers a computationally viable approach to do this in the framework of the FD-TD method. However, our approach can be applied to any computational electromagnetics code that solves the time-domain Maxwell system in its differential form.

Previous research on the incorporation of the Cole–Cole dielectric model in the FD-TD method [13,14] has resulted in schemes of unknown numerical stability and accuracy properties. Recently, a procedure to approximate the H–N dielectric with exponentials in the time domain has been presented [15]. In this work the H–N dielectric model is approximated by Debye functions (poles) in the frequency domain with a preset accuracy over a specified band of frequencies. Therefore the overall scheme in [15] possesses the stability and accuracy properties of the schemes typically used to implement the Debye dielectric model in the FD-TD scheme [16]. However, due to the band-limited nature of the approximation, the polarization dynamics are not accurately represented in the time-domain with a preset accuracy over a specified (and likely long) computational time interval $t \in [0, T_{comp}]$. Further, the singularity of the time-domain susceptibility that arises from dielectric models with fractional relaxation is not taken into account. Consequently, the ability to compute the impulse or step response of spatially complex dispersive scatterers is lost.

It appears that there would be great utility in being able to implement the H–N dielectric model in a way that offers the modeler the ability to perform time-domain simulations over a specified time interval $[0, T_{comp}]$ while maintaining both a preset accuracy for the polarization dynamics and the stability and accuracy attributes of the FD-TD method. Also, it would be desirable that the implementation does not depend on the values of $\alpha$ and $\beta$ thus eliminating the need for separate codes when considering the H–N model's subclasses in the FD-TD method. Although the Debye case ($\alpha \to 1, \beta = 1$) is a singular limit of the H–N model, and thus our approach presented below does not include it, we offer a work-around this shortcoming in the Summary Section 6. Finally, it should be emphasized that it is desirable that the implementation of the polarization dynamics of the HN model be correct at $t = 0^+$ in order to allow the modeler to compute the impulse- or step-response of a spatially complex time-dispersive object directly in the time-domain for the purpose of storing the obtained results at desired spatial locations and later using them to compute the response of the object to arbitrary incident pulses without recomputing with the FD-TD method.

In Section 2 of the paper we present an approach that approximates the induced polarization dynamics of the H–N model with a preset accuracy over an arbitrary (but a priori known) computational time interval $T_{comp}$. We show our method correctly captures both the short- and long-time behavior of the corresponding time-domain susceptibility. The conventional approach to convolution requires $O(N)$ storage, where $N$ is the number of time steps, so that longer computations become progressively restrictive due to memory allocation. In the development of our method we employ the efficient numerical techniques of [17,18] to drastically reduce the required storage from $O(N)$ to $O(\log N)$ in order to compute a convolution and solve the H–N model as a system of $M = \log N$ evolution equations appended to the Maxwell system which requires only the information from the previous time step to perform an update. In Sections 3 and 4 we show our scheme preserves the second order convergence rate and the CFL stability condition of the FD-TD method, and analyze the phase error of our scheme. We close the paper with numerical validations and experiments in Section 5, and a short summary and discussion in Section 6.

2. The numerical scheme

For simplicity, we present our numerical implementation of the H–N model by considering a one-dimensional half-space, $x > 0$, containing a nonmagnetic material ($\mu_0$ is the permeability of vacuum) whose spatially homogeneous dielectric permittivity is given by (1). The proceeding methods can be trivially extended to models with additional terms (i.e., those with multiple H–N terms) and to higher dimensions. Signaling data is prescribed by setting the electric field $E(0, t)$.

We proceed by scaling the space, time and field variables

$$E \rightarrow \sqrt{\varepsilon_0} E, \quad P \rightarrow \frac{1}{\sqrt{\varepsilon_0}} P, \quad H \rightarrow \frac{1}{\sqrt{\mu_0}} H, \quad t \rightarrow T_p t, \quad x \rightarrow \frac{T_p x}{\sqrt{\varepsilon_0 \mu_0}}$$

and the time scale $T_p$ is usually (but not necessarily) chosen to be the dielectric model central relaxation time $\tau$. Maxwell’s equations then become

$$\frac{\partial H}{\partial t} = \frac{\partial E}{\partial x}, \quad \frac{\partial}{\partial t} (\varepsilon_\infty E + P) = \frac{\partial H}{\partial x},$$

where the induced polarization $P$ is defined by the convolution

$$P(x, t) = \int_0^t \chi(t - t') E(x, t') dt'; \quad t > 0.$$  

In Eq. (3) the susceptibility $\chi(t)$ expresses the induced polarization dynamics and for the H–N model it is obtained as the inverse Laplace transform.
\[
\chi(t) = \mathcal{L}^{-1}\left\{ \frac{e_s - e_\infty}{(1 + (st)^{\gamma})^2} \right\} = \frac{\Delta \kappa}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^{st}}{(1 + (st)^{\gamma})^2} ds = \frac{\Delta \kappa}{\pi} \int_0^\infty \frac{\sin(\theta(y)) e^{-\gamma y/t}}{(y^{2\gamma} + 2 \cos(\pi t y^\gamma) + 1)^{\beta/2}} dy
\]

with \(\theta(y) \in [0, \pi \gamma]\) given by
\[
\theta = \cos^{-1}\left\{ \frac{y^\gamma \cos(\pi t) + 1}{\sqrt{y^{2\gamma} + 2 \cos(\pi t) y^\gamma} + 1} \right\}.
\]

This definition will hold in general for \(0 < \gamma < 1\), and is thus valid for both the C–C and H–N models. The C–D model requires a slightly modified treatment; in this case the Bromwich contour used in the inverse Laplace transform is deformed onto the branch cut which is now located along the negative real axis issuing from the branch point at \(s = -1/\gamma\) rather than at the origin (as in the case of the H–N and C–C models). Furthermore, \(\theta \rightarrow \pi\), and the denominator also becomes simplified. We thus obtain the time-domain susceptibility for the C–D model
\[
\chi(t) = \frac{\Delta \kappa}{\pi} \int_0^\infty \frac{\sin(\pi t y)}{(y - 1)^b} e^{-\gamma y/t} dy = \frac{\Delta \kappa}{\pi} \sin(\pi t y) e^{-\gamma y/t} \int_0^\infty y^{-\beta} e^{-\gamma y/t} dy = \frac{\Delta \kappa}{\pi} \left( \frac{t}{\tau} \right)^{b-1} e^{-t/\tau}.
\]

Notice that we can directly evaluate the case \(\beta = 1\) in this latter expression and recover the Debye case; this could also have been done by observing that in this case the distribution in (4) will collapse into a delta function \(\delta(t - \tau)\), which ultimately leads to the same result. The integral in Eq. (5) provides implicitly an integral transform for the singular portion of the susceptibility \(e^{-\gamma y/t}\); through this relation the C–D model can be similarly treated along with the general H–N model.

Specifically, Eqs. (4) and (5) comprise a continuous distribution of exponentials; in fact the Debye case is a “distribution” of a single exponential. The nucleus of our method is to replace the susceptibility by an approximation that makes discretization simple, but for which we have an a priori error bound that is uniform over our computational window \(t \in [0, T_{\text{comp}} = N \Delta t]\). For FD-TD methods, we will use a uniform grid in time that locates the \(E\) and \(P\) fields at \(t_n = n \Delta t\), \(n = 1, 2, \ldots, N\).

To motivate our approximation, we obtain the behavior of the susceptibility by expanding the integrand in (4) for large and small arguments of the integration variable \(y\). Doing so provides the leading order behavior for small and large \(t\) respectively in the H–N case; the corresponding result for the C–D model can be obtained from direct examination of the closed form obtained from Eq. (5). The resulting behaviors for small and large time in each model are:
\[
\chi \sim \begin{cases} t^{\beta - 1}, & t \to 0; \quad t^{-\gamma - 1}, & t \to \infty; \quad H-N, \\ t^{\beta - 1}, & t \to 0; \quad t^{-\gamma - 1}, & t \to \infty; \quad C-C, \\ t^{\beta - 1}, & t \to 0; \quad e^{-t/\tau}, & t \to \infty; \quad C-D. \end{cases}
\]

Recalling that \(0 < \alpha, \beta < 1\) it follows that \(\chi(t) \in L^1([0, c])\) and \(\chi(t) \in L^2([c, \infty])\) for \(c > 0\). Due to the singularity at \(t = 0\), we treat the interval \([0, \Delta t]\) separately. Away from \(t = 0\), \(\chi(t)\) is a smooth algebraically decaying function that can be approximated efficiently with a sum of exponentials over a finite interval \([\Delta t, T_{\text{comp}}]\). Therefore, we will represent the induced polarization as a sum of a local and a history part [19].

\[
P(x, t) = \int_0^t \chi(t - t') E(x, t - t') dt' = \int_0^t \chi(t') E(x, t - t') dt' + \int_0^t \chi(t'') E(x, t - t'') dt'' = P_{\text{loc}}(x, t) + P_{\text{hist}}(x, t).
\]

### 2.1. The local approximation

In order to represent the local part \(P_{\text{loc}}\) of the induced polarization accurately we obtain an asymptotic expansion of the susceptibility \(\chi\) for the small \(t\), of which the leading order behavior is indicated in (6). A simple scaling argument shows that this will correspond to large values of the integration variable \(s\) in the first line of Eq. (4). The Laurent expansion of \(1/(1 + (sx)^\gamma)^2\) is then integrated term by term, resulting in
\[
\chi(t) \approx \frac{\Delta \kappa}{\tau} \sum_{k=0}^K \frac{(-1)^k}{\Gamma(k + \beta)} \left( \beta + k - 1 \right) \left( \frac{t}{\tau} \right)^{(k + \beta) - 1},
\]
where
\[
\left( \beta + k - 1 \right) \left( \frac{t}{\tau} \right)^{(k + \beta) - 1} = \frac{\Gamma(\beta + k)}{\Gamma(k + 1)}
\]
is a generalized binomial coefficient, and the number of terms \(K\) to be included can be determined for a preset precision level.

The C–C and C–D models can be obtained by setting \(\beta = 1\) respectively; for the C–D model, we can see that the expansion is in fact that of the exponential obtained in (5) which is multiplied by the singular term \((t/\tau)^{\beta - 1}\), which means that the expression is exact for \(k \to \infty\). This is true for the H–N model, since the series in (8) can be shown to be absolutely
convergent. Since $\chi \in L_1([0, \Delta t])$, if we assume that $E \in L_2([0, \Delta t])$ then the same will hold for the local approximation $P_{loc}$. We now use linear interpolation to approximate

$$E(x, t - t') \approx E(x, t) + \frac{t'}{\Delta t}[E(x, t - \Delta t) - E(x, t)],$$

which expresses $E$ at the grid points and is second order accurate for $t \in [0, \Delta t]$. The local approximation is then determined to be

$$P_{loc}^n = E^n\left(\int_0^{\Delta t} \left(1 - \frac{t'}{\Delta t}\right) \chi(t')dt'\right) + E^{n-1}\left(\int_0^{\Delta t} \frac{t'}{\Delta t} \chi(t')dt'\right) = \Delta t(\alpha E^n + b E^{n-1}),$$

where

$$a = \sum_{k=0}^{K} \frac{(-1)^k}{\Gamma(\alpha(k + \beta) + 2)} \left(\frac{\beta + k - 1}{k}\right) h^{\alpha(k + \beta)},$$

$$b = \sum_{k=0}^{K} \frac{(-1)^k \alpha(k + \beta)}{\Gamma(\alpha(k + \beta) + 2)} \left(\frac{\beta + k - 1}{k}\right) h^{\alpha(k + \beta)},$$

and $h = \Delta t/t$. We have used the shorthand notation $E^n = E(x, n\Delta t)$. Since we must choose $\Delta t$ small enough to resolve the relaxation time $[16]$, we will have $h < 1$. Furthermore, the coefficients $a$ and $b$ can be also be shown to be absolutely convergent series. To assess the nature of the coefficients for large $k$ we can use Sterling’s approximation generalized for the Gamma function

$$\Gamma(z) = \sqrt{2\pi} \left(\frac{z}{e}\right)^z \left(1 + O(z^{-1})\right)$$

and the binomial coefficient

$$\binom{z + k}{k} = \frac{k^z}{\Gamma(z + 1)} \left(1 + \frac{z(z + 1)}{2k} + O(k^{-2})\right).$$

The terms in the coefficient $b$ will then be of the form

$$b_k = \frac{\alpha(k + \beta)}{\Gamma(\alpha(k + \beta) + 2)} \left(\frac{\beta + k - 1}{k}\right) \approx \frac{\alpha(k + \beta)}{\Gamma(\alpha(k + \beta) + 2)} \frac{k^{\beta-1}}{\Gamma(\beta)} \left(1 + \frac{\beta(\beta - 1)}{2k}\right) \approx \frac{\alpha(k + \beta)}{\Gamma(\beta)} \left(\frac{e}{\sqrt{2\pi}}\right) (\frac{e}{2\beta k})^{\alpha(k + \beta)} \approx C(\alpha, \beta) \left(\frac{e}{2\beta k}\right)^{\alpha(k + \beta) - \beta + 1/2}.$$  

In this final expression, $C(\alpha, \beta)$ is independent of $K$, and is $O(1)$, while the parenthetical term will exhibit exponential decay for $k > e/\alpha$; but since the terms in Eq. (11) are of the form $k^b h^{(K+b)}$, the final term obtained by setting $k = K$ will be sufficiently small for $K$ satisfying $K > he/\alpha$. Upon multiplying the expression (12) by $h^{\alpha(K+b)}$, we obtain the approximate form of the final term in the sum (11), which we set equal to some user-prescribed tolerance $\delta_k$. That is,

$$\delta_k = C(\alpha, \beta) \left(\frac{e h}{2K}\right)^{\alpha(K + \beta) - \beta + 3/2} h^{-3/2} = C \left(\frac{e h}{2K}\right)^{\alpha(K + \beta) - \beta + 3/2}.$$ 

and upon taking the natural log of both sides we have

$$\log \delta_k = (\alpha K + 3/2 - (1 - \alpha)\beta) \log \left(\frac{e h}{2K}\right) + \log C \approx \alpha K \log h + O(1).$$

The discarded terms involving $K$ assuredly remain small, since we consider $K > he/\alpha$. We can now solve the reduced expression for $K$ by omitting the $O(1)$ terms, resulting in a loose upper bound for the number of terms required for convergence,

$$K = \left\lfloor \log \frac{\delta_k}{\alpha \log h} \right\rfloor.$$  

The same bound will hold trivially for $a$ in Eq. (10), since $|a_k| < |b_k|$ for each $k$. Generally $K$ will be relatively small, and in practice $K < 10$ is sufficient to converge to double precision for any values of $0.5 < \alpha, \beta \leq 1$ and $0.0001 < h < 0.01$. It also follows from the restriction on $K$ that fewer terms are required for smaller values of $h$, and larger $\alpha$. In the present context, the linear interpolation of the electric field will introduce a second order error, so if we choose $\delta_k < h^2$ we are assured that the local approximation will maintain second order accuracy.
2.2. The history approximation

The kernel of the history part in (7) is now approximated as follows

\[ \left| \chi(t) - \frac{\Delta e}{\tau} \sum_{j=1}^{M} w_j e^{-y_j/(\tau t)} \right| < \delta_M, \tag{14} \]

where \( \delta_M \) is again a user-prescribed tolerance, and the norm is defined to be

\[ \| \cdot \| = \max_{\Delta t \leq t \leq \Delta T} \| \cdot \|. \]

The values of the weights and nodes \( \{w_j, y_j\} \) are determined using generalized Gaussian quadrature [17]. Such quadrature weights and nodes can be obtained in several different ways; Beylkin et al. has designed a scheme for finding a sum-of-exponentials approximation for a given function [18]. In that work, it is indicated that for a smooth function (which we have, on \([\Delta t, T_{\text{comp}}]\)) the number of nodes can be minimized using the error tolerance, resulting in \( M = O(\log 1/\delta_M + \log N) \). Alternatively, if we define \( \chi(t) \) by a contour integration we can use the methods originally proposed by Rokhlin et al. [20]. Finally, one can take the Laplace transform of \( \chi(t) \), and use it to find a sum-of-poles approximation, then invert this latter expression.

In the present work, we proceed by making the substitution \( x = \tan \theta / \pi \) in Eq. (4), which maps the integrand to a finite domain \( 0 < x < \pi / 2 \); we then find a generalized gaussian quadrature in the variable \( 0 \). Since (14) has to be satisfied for all \( t \in [\Delta t, N \Delta t] \), we will sample the interval \([\Delta t, N \Delta t] \) by \( P \gg N \) points \( t_p, p = 1, \ldots, P \) and force (14) to be satisfied at these \( P \) discrete points. Recall now that each \( \chi(t_p) \) is represented as a finite integral on a fixed interval with different integrand functions \( t_p \) here is acting as a parameter (or index) for these \( P \) functions \( f_p \). However, the crucial observation is that these \( P \) functions \( f_p \) are not linearly independent numerically. Indeed, by performing a SVD on these \( P \) functions, there are only about \( 2M = O(\log 1/\delta_M + \log N) \) linearly independent basis functions \( g_m \), \( m = 1, \ldots, 2M \) above the threshold \( \delta_M / 100 \) (in our actual computation, \( P = 200,000 \), and \( 2M = 86 \)). Finally, we apply the generalized Gaussian quadrature [18,20] on these \( 2M \) basis functions and obtain a sum-of-exponential approximation with only \( M \) nodes and weights. Once the weights and nodes are obtained, we define the history part of the induced polarization

\[ P_{\text{hist}} = \frac{\Delta e}{\tau} \int_0^{t - \Delta t} \sum_{j=1}^{M} w_j e^{-y_j/(\tau t')} E(x, t') dt' = \sum_{j=1}^{M} w_j \phi_j, \]

where the auxiliary functions satisfy a recurrence relation (viz. \( t_{n+1} = (n + 1) \Delta t \)),

\[ \phi_j^{n+1} = \frac{\Delta e}{\tau} \int_0^{n \Delta t} e^{-y_j/(\tau [n - \Delta t - t'])} E(x, t') dt' = \frac{\Delta e}{\tau} e^{-y_j/\tau} \left( \int_0^{(n-1) \Delta t} + \int_{(n-1) \Delta t}^{n \Delta t} \right) e^{-y_j/(\tau [n - \Delta t - t'])} E(x, t') dt' \]

\[ = e^{-y_j/\tau} \phi_j^n + \frac{\Delta e}{\tau} e^{-y_j/\tau} \int_0^{\Delta t} e^{-y_j/\tau} E(x, n \Delta t - t') dt'. \tag{15} \]

We point out here that while \( \phi_j \) can also be described using differential equations, these equations will be stiff, since typically \( y_j \in [10^{-3}, 10^{3}] \). Similarly for the weights we have \( w_j \in [10^{-5}, 10] \); Fig. 1 shows a typical distribution of weights and nodes that arise in our problem for \( T_{\text{comp}} = 300 \).

Fig. 1. A typical distribution of Gaussian weights and nodes for the susceptibility \( \chi \). The quadrature is designed using \( \Delta t = 5 \times 10^{-4} \), and \( \delta_M = 10^{-9} \) for \( \alpha = \beta = 0.75 \).
Conversely, this method can be equivalently derived using exponential time differencing [21]. This final integral can be computed directly if we again approximate $E$ with its linear interpolant across one time step (9), which results in

$$
\phi_j^{n+1} = e^{-\gamma_j h} \phi_j^n + \Delta \epsilon \left( c_j E^n + d_j E^{n-1} \right),
$$

from which, after making a substitution $t' = ut$, we obtain

$$
c_j = e^{-\gamma_j h} \int_0^h \left(1 - \frac{u}{h}\right) e^{-\gamma_j u} du = \frac{e^{-\gamma_j h}}{y_j^2 h} \left( (e^{-\gamma_j h} - 1 + y_j h) \right),
$$

$$
d_j = e^{-\gamma_j h} \int_0^h \frac{u}{h} e^{-\gamma_j u} du = \frac{e^{-\gamma_j h}}{y_j^2 h} \left[ (1 - e^{-\gamma_j h}(1 + y_j h)) \right].
$$

(16)

2.3. The numerical scheme

Finally, we combine the local and history parts and present the full numerical scheme using the staggered space–time mesh of the FD-TD method. We compute $E$ and $P$ at the nodes $(x_m, t_n) = (m\Delta x, n\Delta t)$, and $H$ at the corresponding semi-nodes. This results in the following discrete form of the equations in (2),

$$
\frac{H^{n+1/2}_{m+1/2} - H^{n-1/2}_{m+1/2}}{\Delta t} = \frac{E_{m+1}^n - E_m^n}{\Delta x},
$$

$$
\frac{\epsilon_{\infty} E_{m+1}^n - E_m^n + P_{m+1}^n - P_m^n}{\Delta t} = \frac{H_{m+1/2}^{n+1/2} - H_{m-1/2}^{n+1/2}}{\Delta x},
$$

which are closed with the discretized induced polarization law (3)

$$
P_{m+1}^n = \Delta \epsilon \left( a E_{m+1}^n + b E_m^n \right) + \sum_{j=1}^{M} w_j \phi_{jm}^{n+1},
$$

$$
\phi_{jm}^{n+1} = e^{-\gamma_j h} \phi_j^n + \Delta \epsilon \left( c_j E_m^n + d_j E^{n-1}_m \right), \quad j = 1, 2 \ldots M.
$$

3. Stability analysis

We now study the stability of the scheme by constructing the Von Neumann polynomial. Our goal is to determine whether or not the usual CFL stability condition for the FD-TD method also holds for our scheme. Let

$$
\left( H_{m+1/2}^{n+1/2}, E_m^n, P_m^n, \phi_{1m}^{n+1}, \ldots \phi_{Mm}^{n+1} \right)^T = U \rho^{n} e^{i\omega n \Delta x}.
$$

The time index has been shifted for $H$ and $[\phi_j]$ for convenience, and will not change the resulting polynomial. Upon substituting into each equation we solve for the characteristic polynomial

$$
\Phi(\rho) = \prod_{k=1}^{M} (\rho - e^{-\gamma_j h}) \left( \Phi_1(\rho) + \frac{\Delta \epsilon}{\epsilon_{\infty}} \Phi_2(\rho) \right) = 0,
$$

where

$$
\Phi_1 = \rho \left[ \rho^2 - 2 \left( 1 - 2 v^2 \sin^2 \left( \frac{k\Delta x}{2} \right) \right) \rho + 1 \right],
$$

$$
\Phi_2 = \left( \rho - 1 \right)^2 \left[ a \rho + b + \sum_{j=1}^{M} w_j \frac{c_j \rho + d_j}{\rho - e^{-\gamma_j h}} \right],
$$

$v = c_{\infty} \Delta t / \Delta x$ is the CFL number, and $c_{\infty} = 1 / \sqrt{\epsilon_{\infty} \mu_0}$ is the maximum phase velocity in the H–N medium. While $\Phi_2$ is not strictly a polynomial, the denominator terms will cancel when the product is expanded; consequently, $\rho = e^{-\gamma_j h}$, $j = 1, 2 \ldots M$ will not be eigenvalues of the numerical scheme in general. Although compactly written, $\Phi(\rho)$ is in fact the addition of $M + 2$ polynomials of degree $M + 3$.

Before characterizing the general behavior of the roots, we first examine a few important limiting cases. When $\Delta \epsilon \to 0$, we see that $\Phi_2$ vanishes. Thus, the roots can be determined analytically as
\[ \rho = \{ 0, \epsilon^i, e^{-i\epsilon}, e^{-\gamma h}, \ldots, e^{-\gamma nh} \}, \]

where the substitution \( \sin \frac{\pi}{2} = \frac{v}{w} \sin \frac{\pi k}{2w} \) is used to define the modes of interest. When \( v > 1 \), there will be a wave number \( k' \) for which \( v \sin \frac{\pi k'}{2w} = 1 \). For \( k > k', \tilde{\xi} \) will become complex resulting in one of the roots leaving the unit circle; that is, instability.

For \( v \leq 1 \), the roots will both traverse the unit circle from \( \rho = 1 \) when \( k = 0 \), and move to \( \rho = e^{i\theta} \) when \( k\Delta x = \pi \), where \( \sin \frac{\pi}{2} = \frac{v}{w} \). The remaining modes are stationary for all values of \( k\Delta x \), and are simple zeros that lie along the positive real axis and will cluster at the origin for larger values of \( y/h \). The polynomial will be a Schur polynomial [22], leading immediately to stability.

Next we examine the ratio \( r = \epsilon w, e^w \rightarrow \infty \); as \( r \) becomes large we may neglect \( \Phi_1 \), but must now deal with a polynomial of degree \( M + 3 \), where the none of the roots are easily tractable, except the obvious root of multiplicity 2 at \( \rho = 1 \). Focusing on the remaining polynomial, we wish to think of the roots as being perturbed from some value that is nearly a root of the polynomial. This happens, for instance when the summation is expanded, and \( \rho = e^{-\gamma h} \) is a zero of all but one of polynomials in the summation. We thus make use of a standard result in perturbation theory [23]:

Consider a polynomial \( \Phi(\rho) = P(\rho) + cg(\rho) \), where \( \rho_0 \) is a root of \( P(\rho) \) but not of \( g(\rho) \). Then, if \( \rho(\epsilon) = \rho_0 + \epsilon \rho_1 + \cdots \) is a root of \( \Phi(\rho) \), we have \( \rho_1 = -g(\rho_0)/f(\rho_0) \), which is well-behaved if \( f(\rho_0) \) is bounded away from 0. Now for \( \rho_0 = e^{-\gamma h} \)

\[
f(\rho) = P(\rho) \left( a\rho + b + \sum_{j=1}^{M} w_j \frac{c_j\rho + d_j}{\rho - e^{-\gamma h}} \right) (\rho - e^{-\gamma h}),
\]

\[
g(\rho) = P(\rho) (c_i\rho + d_i),
\]

where

\[
P_\ell(\rho) = (\rho - 1)^2 \prod_{k=\ell}^{M} (\rho - e^{-\gamma h})
\]

and \( \epsilon = w \). We can now see that indeed \( \rho_0 = e^{-\gamma h} \) is a root of \( f \) but not of \( g \). A simple calculation gives

\[
g(\rho_0) = P_i(e^{-\gamma h}) (c_i e^{-\gamma h} + d_i),
\]

\[
f'(\rho_0) = P_i(e^{-\gamma h}) \left( ae^{-\gamma h} + b + \sum_{j=1}^{M} w_j \frac{c_j e^{-\gamma h} + d_j}{e^{-\gamma h} - e^{-\gamma h}} \right).
\]

Thus, \( e^{-\gamma h} \) will be perturbed to first order by an amount

\[
\rho = \rho_0 - w_i \frac{g(\rho_0)}{f'(\rho_0)} = e^{-\gamma h} \left( 1 - \frac{w_i (c_i e^{-\gamma h} + d_i)}{(ae^{-\gamma h} + b + \sum_{j=1}^{M} w_j \frac{c_j e^{-\gamma h} + d_j}{e^{-\gamma h} - e^{-\gamma h}})} \right).
\]

![Fig. 2. Motion of the roots for varying values of \( k\Delta x \). When \( r = \frac{1}{r} \) is small, the roots traverse arcs that approach the unit circle. As \( r \) increases, these arcs decrease in magnitude, so the roots always remain inside the unit disk. The values along the real axis remain nearly stationary for all \( k\Delta x \), and will not leave the unit disk.](image-url)
The second term will always be small and positive. For the weights and nodes corresponding to Fig. 1, the right term will vary by several orders of magnitude, but remain small as $O(10^{-6}, 10^{-2})$. The larger values of $y_j$ will correspond to a more pronounced contraction from the value $p_0$; for smaller $y_j$ the roots barely change. A numerical investigation has confirmed these results; for various values of $r$ and $k\Delta t$, the roots all remain on the positive axis and are contained in the unit disk. Similarly, one can show that a root near the origin arises from the coefficients $a$ and $b$, which will remain on the negative axis, and is bounded below by $-b/a > -1$; as $r \rightarrow 1$ ($\Delta \epsilon \rightarrow 0$), this root becomes the zero eigenvalue in (17).

Finally the double root at $\rho = 1$ will be perturbed and become two complex conjugate roots whose motion is contained in the first and fourth quadrants, respectively. The motion of these roots is illustrated for several values of $r$ in Fig. 2. Recall, as $r \rightarrow \infty$, these roots coalesce at $\rho = 1$, and they will only remain on the unit circle in the case $r = 1$, or equivalently $\Delta \epsilon = 0$. Thus, we have shown that all roots are contained within the unit disk for $m > 1$, and stability follows immediately.

4. Phase error analysis

In general there will be two sources of error in computing a numerical solution to the system (2): the error incurred when approximating the susceptibility $\chi(t)$ for $t \in [0, T_{\text{comp}} = N \Delta t]$, and the typical local truncation error of the FD-TD method. The discretization we presented in Section 2 allows full control of the first kind of error that arises from both the local and history part of the polarization law (3). This is done by first prescribing the precisions $\delta_K$ and $\delta_M$ for the local and history portions respectively; then choosing $K$ according to (13) and finding the minimum number of terms $M$ which satisfies (14). As long as we set $\delta_K, \delta_M < h^2$ then we are assured that the error introduced over the computational time interval $T_{\text{comp}}$ by the polarization will be smaller than the local truncation error in time for the FD-TD method. The results shown below will hold for the implementation of the H–N, C–C and C–D models.

We study the phase error of our scheme by analyzing the numerical dispersion relation. The numerical wave number $k_h^K, (\omega)$ satisfies

$$ k_h^K (\omega) = \frac{\omega}{c_h^K} $$

Fig. 3. The phase error decreases for smaller values of $h = \Delta t/r$, which is the dominant source of error made in computing the solution; that is, the error due to the discretizing the convolution is negligible.
\[ \sin^2 \left( \frac{k^2 h M \Delta x}{2} \right) = \frac{1}{2} \left( \frac{1}{\sqrt{2}} \right) \left[ 1 + \frac{k^2}{k^2 + \gamma_k^2} \right] \]

where

\[ \gamma_k^2 = \left( \frac{\tau_k}{\tau} \right)^2 \left( 1 + (i \tau)^\beta \right) \]

is the scaled susceptibility (with \( \Delta \varepsilon = 1 \)). The phase error \( \Phi_h = |\Phi_h - 1| \) is plotted for several values of \( h = \Delta t/\tau \) in Fig. 3; the quadrature used in each case is the same, and is designed with \( \delta_k = \delta_M = 10^{-5} \) and \( \Delta t = 5 \times 10^{-4} \); thus the quadrature should maintain accuracy for \( \Delta t > 5 \times 10^{-4} \). Fig. 3 validates this assertion, and shows that the error observed is comprised predominantly of the discretization error. If \( \Delta t \) is decreased past the value for which the quadrature is designed, then the quadrature error will eventually dominate the total error, and further decreasing the step size will not improve the overall accuracy.
We now show the phase error is second-order accurate in $\Delta t$ and $\Delta x$. Using the definitions of $a$ and $b$ in Eqs. (10) and (11), it can be easily shown that

$$a + be^{i\omega \Delta t} = \int_0^{\Delta t} \chi(t')L(e^{i\omega \Delta t})dt' + O(\delta \epsilon + \Delta t^2),$$

where $\chi(t)$ is approximated using the small time expansion in (8), and

$$L(e^{i\omega \Delta t}) = 1 + (e^{i\omega \Delta t} - 1) \frac{t'}{\Delta t}$$

is the linear interpolant of $e^{-i\omega t}$ over the interval $[0, \Delta t]$. Similarly, the history portion can be rearranged by invoking the definitions (16) of the coefficients, and making use of a geometric series to show that

$$\sum_{j=1}^{M} w_j \frac{c_{j} e^{i\omega \Delta t} + d_{j} e^{-2i\omega \Delta t}}{1 - e^{-(y_j h + i\omega \Delta t)}} = \sum_{j=1}^{M} w_j \left( \int_0^R \left( 1 - \frac{u}{h} + \frac{u}{h} e^{-i\omega \Delta t} \right) e^{-(y_j h + i\omega \Delta t)} du \right) \sum_{n=0}^{\infty} e^{-(y_j nh + i\omega \Delta t)}$$

$$= \int_0^{\Delta t} L(e^{i\omega \Delta t}) \sum_{n=0}^{\infty} e^{-i\omega(n+1)\Delta t} \sum_{j=1}^{M} w_j e^{-y_j nh / \tau} dt' / \tau$$

$$= \sum_{n=1}^{\infty} e^{-i\omega \Delta t} \int_0^{\Delta t} L(e^{i\omega \Delta t}) \chi(t' + n\Delta t) dt' + O(\delta \epsilon).$$

**Fig. 5.** Validation of the Havrilak–Negami model. The program requires no augmentation to run the C–C and H–N models.
Recall that $\delta_M$ is the prescribed error used to define the generalized Gaussian nodes, and is therefore the error made in replacing the sum with the true susceptibility. We now make use of the fact that the contribution from $a$ and $b$ in (18) is precisely the $n=0$ summand, which we combine to obtain

$$
\hat{j}_b^{KM}(\omega) \approx \sum_{n=0}^{\infty} e^{-i\omega n\Delta t} \int_0^{\Delta t} L(e^{-i\omega t}) \chi(t' + n\Delta t) dt' + O(\delta_k + \delta_M) = \sum_{n=0}^{\infty} \int_{n\Delta t}^{(n+1)\Delta t} \chi(t') e^{-i\omega t'} dt' + O(\delta_k + \delta_M + \Delta t^2),
$$

which is immediately recognized as a second order accurate approximation to the Fourier transform $\hat{j}$, as is desired. This shows explicitly that for a given choice of $\delta_k$, $\delta_M < O(\Delta t^2)$, we maintain the second order accuracy of the FD-TD method.

5. Numerical validation and experiments

The solution to the systems (2) and (3) was computed for signalling data comprised of short-duration pulses and for various values of $(\alpha, \beta)$. The electric field at $x = 0$ is a square impulse of duration $t_d = \tau/100$ (short pulse) or $t_d = \tau$ (long pulse), both with unit area. Time traces were recorded at several spatial locations in order to observe the solution. The simulations are terminated prior to the signal reaching the right-hand boundary, so that no reflection is encountered.

We first present a validation of our scheme. In these validations, the exact electric field is calculated independent of the FD-TD scheme, through a numerical evaluation of the inverse Laplace transform, as follows:

$$
E_{\text{exact}}(x, t) = \int_0^t E(0, t') G(x, t - t') dt',
$$

Fig. 6. Validation of the Cole–Davidson model at small (left) and large (right) depths for $t \in [0, 100]$. 

Fig. 7. Convergence of $L_2$ error over the time interval $[0, 300]$ at (from left to right) $x = 0.008$, $x = 1$ and $x = 10$. 
where

\[ G(x, t) = \mathcal{L}^{-1}\{e^{[-(t-x/C_0)]}\}; \quad t > 0 \]

is the Green's function for the H–N medium, and \( c(s) = c_0/\sqrt{\epsilon(s)} \) is given in terms of the permittivity (1) with \( s = \imath \omega \). We must point out here that the exact solution is obtained using different methods of quadrature on the inverse Laplace transform \( G(x, t) \), depending on whether a small or large depth solution is sought. The number of quadrature points are increased until a level of accuracy that is better than the most accurate FD-TD simulation is achieved, so that for all practical purposes, we may call these computations “exact”. The optimal choice of the Bromwich contour, quadrature weights and nodes, as well as the associated numerical parameters for evaluating \( G(x, t) \) will be reported elsewhere.

The solution will exhibit characteristically different behavior at short and large distances away from the left boundary, \( x = 0 \), of the dielectric half-space; thus we show a validation for each of these spatial regions. The C–C model is validated in Fig. 4, and the H–N model in Fig. 5. In both instances the numerical solution is computed with the same code; the only change is in the parameters \( \alpha \) and \( \beta \). This demonstrates that our method can treat both of these dielectric models. When computing the C–D model, we have to change the quadrature accordingly as shown in (5); this augmented scheme is validated in Fig. 6. In all three cases, the agreement is very good.

We next consider the \( L^2 \) error, computed over the computational time interval \( T_{\text{comp}} = 300 \), with respect to the exact solution, (19), of our model problem. The convergence of this error is plotted in Fig. 7 for several values of \( h = \Delta t/\tau \), and \( \alpha = \beta = 0.75 \), at a range of depth spanning four orders of magnitude. The values of these curves are plotted on a log–log scale, and show second order accuracy. The observed convergence rate holds independently of \( \alpha \), \( \beta \), and for the C–C and C–D models as well.

In Section 2, it was shown that for short times, the behavior of the susceptibility was determined as \( \chi \sim t^{\alpha \beta - 1}, t \to 0^+ \). This indicates that for different values of \( \alpha \) and \( \beta \) we would expect similar short time behavior in the electric field if the product of these is close; this is demonstrated in Figs. 8 and 9, for the long and short duration pulses, respectively. Despite the fact that the

![Fig. 8. A typical short-depth electric field for a Cole–Cole (left) and Havriliak–Negami (right) medium. The transient behavior is very much the same, since the product \( \alpha \beta \) is nearly the same for both media. The initial pulse duration was \( t_0 = \tau = 1 \), with amplitude 1.](image-url)
Fig. 9. For the same two cases, the short-depth plots are shown with a pulse that is of duration $t_d = t/100$ and amplitude 100.

Fig. 10. The $(x,t)$ location of the peak electric field value is traced for the Debye and H–N models. All modeling parameters are the same, except $\alpha$ and $\beta$, $(1,1)$ and $(0.75,0.75)$, respectively. The Debye model undergoes a sudden transition from the ray defined by $c_1$ to that of $c_s$, whereas the transition is smooth in the H–N case.
top plots depict a C–C medium, and the bottom an H–N medium, the electric field is nearly indistinguishable. The waveforms shown here capture the transient behavior of the solution, which occurs in the so called time-domain skin-depth [24]. The initial discontinuities rapidly vanish, which can be confirmed with an asymptotic investigation of the electric field [25]. The long pulse will remain constant for a longer duration, and so its spectrum will contain larger amplitudes in the high-frequency regime. Consequently, the larger frequencies persist longer into the skin-depth for the longer pulse (note the scale of the t-axis). The short pulse more closely approximates a delta function, and so is a good approximation to the impulse response of the material. In this region, the waveforms will travel at the infinite frequency speed, \( c_1 = c_0 / \sqrt{\varepsilon_\infty} \); past the skin-depth we see a transition to the static (zero-frequency) speed \( c_s = c_0 / \sqrt{\varepsilon_s} \), as shown in Fig. 10. While this transition is sudden and clear in a Debye type medium, the transition is smooth in a general H–N, C–C or C–D medium due to the continuous distribution of relaxation times. Beyond this transition region, the susceptibility will be approximated well by \( \chi \sim t^{-\alpha-1}, t \to \infty \).

This behavior is shown in Fig. 11 for the same solutions as shown in Figs. 8 and 9, observed at a deeper spatial location for which \( x = 10 \). Now the transient behavior has subsided, and the solution will be a material response, determined by the dielectric parameters; thus, independent of the shape of the original signal. The amplitude and shape of the electric field are very close between the short and long pulses, despite the disparate starting amplitudes. This is not terribly surprising, since the spectra of the two signals will have very similar low-frequency content. We can also see the effects of \( \alpha \) and \( \beta \) as shaping parameters on these characteristic waveforms, which is illustrated in Fig. 11 by the large depth behavior of the H–N and C–C fields. When \( \alpha \) is increased, the asymmetry and tail of the waveform is increased; decreasing \( \beta \) narrows the waveform, and raises the peak slightly.

6. Summary

In this paper we have developed a novel method to construct time-domain simulations for the family of anomalously dispersive dielectrics represented by the Havriliak–Negami induced polarization model. Specifically we have used the FD-TD
method, and an efficient approximation of the induced polarization convolution using a sum of exponentials arrived at by applying generalized Gaussian quadratures. The convolution kernel is constructed with a preset level of accuracy that is uniform over a predetermined computational window, and can be set below the expected truncation error, so that the overall error is second order as in the FDTD scheme. We explicitly addressed the C–C, C–D and general H–N cases when constructing these approximations, and note here that the Debye model can be incorporated as well, simply by omitting the local portion of the approximation across the first time step (which is unnecessary), and updating the history portion only at the single exponential node \( y = 1 \); this is equivalent to implementing the Debye model using exponential time differencing, or evaluating the recurrence relation as shown in Section 2. We have also shown using Von Neumann analysis that the overall resulting numerical scheme is stable with no additional restriction placed on the time step other than the typical CFL condition. Numerical simulations confirm the stability and accuracy results, and we validate the numerical solutions via alternate representations of the exact solutions using Laplace transforms.

References