Time Domain Parameter Distribution Estimation in Dispersive Media

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Abstract

The Cole-Cole model is known to accurately describe the dielectric response of a dispersive material over a wide range of frequencies. The model, however, does not lend itself easily to fast, efficient time domain simulation methods such as the Finite Difference Time Domain (FDTD) method. Instead the physics-based Debye model (of which the Cole-Cole model is a non-physical, heuristic generalization) is often used. However, simulations do not match data over any broad range of frequencies. In this work, we seek to avoid the difficulty of implementing the Cole-Cole model by presenting an approximation of dispersive mechanisms using distributions of parameters within the Debye model. Thus, parameter estimation becomes an inverse problem for the distribution of dielectric parameters. We formulate and solve this inverse problem in the case of time-domain electric field data. The forward problem requires a fast FDTD implementation capable of incorporating distributions of parameters.

Introduction

A fundamental question in electromagnetics is how to model dispersion and dissipation of the fields in complex materials such as biological tissue. This has most often led to the use of Maxwell's equations coupled with constitutive relationships for polarization. The problem is even more difficult with noisy data or variability (heterogeneity) in the material being interrogated. Some deterministic models have been generalized to an extent that they seem to account for this variability, but there is some question as to whether the resulting models are even physically realistic.

A recently rediscovered modeling framework allows uncertainty at the molecular level through distributions of parameters representing molecular variability. Intensive experimental efforts have been pursued in describing data for complex materials in the frequency domain with distributions of dielectric parameters, especially relaxation times in multiple Debye models. A significant amount of this work is reviewed in the survey paper by Foster and Schwan[5]. The corresponding time-domain inverse problems were initially developed in [1] and examples for a one dimensional case were solved in [2] using finite elements for the forward simulation and quadrature for computing the expected value over a distribution. Our contribution here is to implement a fast forward solver utilizing the generalized Polynomial Chaos framework. This allows use of the finite difference time domain (FDTD) method for solving the dispersive Maxwell's Equations and eliminates the need for a separate computation of expected values.

Maxwell's equations may be coupled with constitutive laws to include effects from polarization

$$\mathbf{D} = \epsilon\mathbf{E} + \mathbf{P}, \tag{1}$$

where $\epsilon = \epsilon_0\epsilon_\infty$. In (1), $\mathbf{D}$ and $\mathbf{E}$ represent the electric flux density and the electric field, respectively; $\mathbf{P}$ is the polarization, ϵ_0, the electric permittivity of free space; ϵ_∞, the electric permittivity in the limit of infinite frequencies. The polarization, written in the convolution form, is

$$\mathbf{P}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\nu)\mathbf{E}(s,\mathbf{x})ds, \tag{2}$$

where $g(t,\mathbf{x})$ is the dielectric response function (DRF) and ν is a set of dielectric parameters. The DRF for a Debye Medium is

$$g(t,\mathbf{x}) = \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau}e^{-t/\tau}, \tag{3}$$

with $\nu = \{\epsilon_s, \epsilon_\infty, \tau\}$. Here ϵ_∞ represents the electric permittivity in the limit of static frequency, and τ is called the relaxation time. The polarization in (2) defined by (3) can be shown to be equivalent to the solution of the ordinary differential equation,

$$\tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0\epsilon_d\mathbf{E}, \tag{4}$$

where $\epsilon_d = \epsilon_s - \epsilon_\infty$.

It is common to assume multiple poles of Debye-type polarization corresponding to multiple mechanisms. Converting to the frequency domain,

$$\hat{\mathbf{D}} = \epsilon(\omega)\hat{\mathbf{E}} \tag{5}$$

the complex permittivity for the multi-pole Debye model is given by

$$\epsilon(\omega)_D = \epsilon_\infty + \sum_{m=1}^{n} \frac{\Delta\epsilon_m}{1+(i\omega\tau_m)} + \frac{\sigma}{i\omega\epsilon_0}, \qquad (6)$$

where each τ_m represents one of the relaxation time parameters, $\Delta\epsilon_m = \epsilon_{s_m} - \epsilon_{s_{m-1}}$ (except for $\Delta\epsilon_1$, since $\Delta\epsilon_1 = \epsilon_{s_1} - \epsilon_\infty$), and n is the number of poles. The conductivity, σ, is assumed to be given by Ohms law. A best fit of Debye model parameters [3] to permittivity data for dry skin is depicted in Figure 1 (see [3] for the imaginary part).

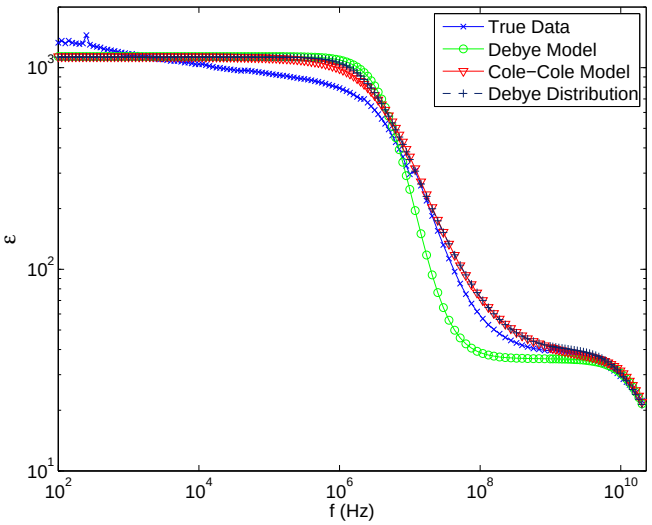

Figure 1: Real part of $\epsilon(\omega)$, ϵ, or the permittivity.

A better fit to data can be achieved by the Cole-Cole model, a heuristic generalization of Debye

$$\epsilon(\omega)_{CC} = \epsilon_\infty + \sum_{m=1}^{n} \frac{\Delta\epsilon_m}{1+(i\omega\tau_m)^{(1-\alpha_m)}} + \frac{\sigma}{i\omega\epsilon_0}, \quad (7)$$

where α_m are non-physical parameters. The fit to dry skin data for the Cole-Cole model is also depicted in Figure 1. The Cole-Cole model does not correspond to a simple ODE in the time-domain, but rather a fractional order differential equation. Therefore parameters determined for this model are not easily used in a forward simulation. Existing options involve discretizing the inverse Laplace transform resulting in methods equivalent to using a multi-pole Debye model for a single dispersive mechanism.

Methods

Distributions

To allow for a distribution F of parameters ν over some admissible set $\mathcal{N}$, we generalize the polarization law (2) to

$$\mathbf{P}(t,\mathbf{x};F) = \int_0^t \int_{\mathcal{N}} g(t-s,\mathbf{x};\nu)\mathbf{E}(s,\mathbf{x})dF(\nu)ds. \quad (8)$$

where F is chosen from the space $\mathcal{F} = \mathfrak{P}(\mathcal{N})$ of all probability measures F on $\mathcal{N}$.

In [3], the inverse problem to determine the distribution of parameters which minimizes some measure of error with complex permittivity data was investigated. In a multi-pole model, each mechanism is modeled by a distribution of parameters, thus requiring discrete combinations of continuous distributions. For example, the best fit to dry skin data using two uniform distribution of dielectric parameters in the multi-pole Debye model is depicted in Figure 1 (labeled Debye Distribution).

Forward Problem

We define the *random polarization* $\mathcal{P}(\mathbf{x},t;\tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d\mathbf{E} \qquad (9)$$

where τ is a random variable with PDF $f(\tau) = dF(\tau)$, for example, $f(\tau) = (\tau_b - \tau_a)^{-1}$ for a uniform distribution. The electric field depends on the macroscopic polarization, defined in (8), which can be shown to be equivalent to the *expected value* of the random polarization

$$\mathbf{P}(\mathbf{x},t;F) = \int_{\tau_a}^{\tau_b} \mathcal{P}(\mathbf{x},t;\tau)f(\tau)d\tau.$$

Existence and uniqueness of solutions to weak formulation of the 1D forward problem, as well as continuous dependence of $(E,\dot{E})$ on F in the Prohorov metric shown in [1].

Inverse Problem for Distributions

Given data $\{\hat{E}\}_j$ we seek to determine a probability measure F^*, such that

$$F^* = \min_{F\in\mathfrak{P}(\mathcal{Q})} \mathcal{J}(F),$$

where, for example,

$$\mathcal{J}(F) = \sum_j \left(E(t_j;F) - \hat{E}_j\right)^2.$$

Continuity of $F \to (E,\dot{E})$ implies continuity of $F \to \mathcal{J}(F)$, for a continuous objective function J. Compactness of $\mathcal{Q}$ implies compactness of $\mathfrak{P}(\mathcal{Q})$ with respect to the Prohorov metric. Therefore, a minimum of $\mathcal{J}(F)$ over $\mathfrak{P}(\mathcal{Q})$ exists [1].

Approximating the Random Polarization

We apply the generalized Polynomial Chaos approach to our random polarization model in order to separate the time dependence from the randomness [6]. We then truncate the expansion in random space resulting in a deterministic, linear system of ordinary differential equations (coupled to Maxwell's Equations) for an approximation to the random polarization. Specifically, in one spatial dimension z, we assume an expansion (at each point in space) in terms of othogonal polynomials $\{\phi_j\}$ given by

$$\mathcal{P}(t;\tau) = \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi),$$

with $\tau = \tau(\xi) = r\xi + m$, e.g., $\xi \sim \text{Beta}(a, b)$. Projecting into a finite dimensional subspace, (9) becomes

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0\epsilon_d E\vec{e_1} =: \vec{g}$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

Maxwell's Equations depend on the macroscopic polarization, the expected value of the random polarization at each point (z, t), which is simply

$$P(z, t; F) = \alpha_0(z, t).$$

and therefore there is no need to include randomness in Maxwell's Equations. In the above,

$$M = \begin{bmatrix} b_0 & a_1 & & & \\ c_0 & b_1 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_p \\ & & & c_{p-1} & b_p \end{bmatrix},$$

where the diagonals come from the coefficients of the triple recursion formula for the choice of family of standard orthogonal polynomials

$$\xi\phi_j = a_j\phi_{j-1} + b_j\phi_j + c_j\phi_{j+1}$$

(with the assumption that $\phi_{-1} = 0$). See [4] for the details of the derivation.

Numerical Simulation of Foward Problem

To solve the inverse problem for the distribution of relaxation times, we need a method of accurately and efficiently simulating $P(z, t; F)$ that is compatible with FDTD for Maxwell's Equations. Applying the central difference approximation, based on the Yee scheme, Maxwell's equations with conductivity and polarization included,

$$\epsilon\frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \sigma E - \frac{\partial P}{\partial t}$$

and

$$\mu\frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z}$$

become

$$\epsilon\frac{E_k^{n+\frac{1}{2}} - E_k^{n-\frac{1}{2}}}{\Delta t} = -\frac{H_{k+\frac{1}{2}}^n - H_{k-\frac{1}{2}}^n}{\Delta z} - \sigma\frac{E_k^{n+\frac{1}{2}} + E_k^{n-\frac{1}{2}}}{2} - \frac{P_k^{n+\frac{1}{2}} - P_k^{n-\frac{1}{2}}}{\Delta t}$$

and

$$\mu\frac{H_{k+\frac{1}{2}}^{n+1} - H_{k+\frac{1}{2}}^n}{\Delta t} = -\frac{E_{k+1}^{n+\frac{1}{2}} - E_k^{n+\frac{1}{2}}}{\Delta z}.$$

Note that while the electric field and magnetic field are staggered in time, the polarization updates simultaneously with the electric field.

Applying second order central differences to $\vec{\alpha} = \vec{\alpha}(z_k)$ gives

$$A\frac{\vec{\alpha}^{n+\frac{1}{2}} - \vec{\alpha}^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}^{n+\frac{1}{2}} + \vec{\alpha}^{n-\frac{1}{2}}}{2} = \frac{\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}}{2}.$$

Combining like terms gives

$$(2A + \Delta tI)\vec{\alpha}^{n+\frac{1}{2}} = (2A - \Delta tI)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t\left(\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}\right).$$

Note that $(2A + \Delta tI)$ is tridiagonal and small (e.g., 8×8). The numerical stability of this method for CFL number $\nu \leq 1$ is established in [4] for the Beta distributions with Jacobi polynomials.

This approach gives a simple and efficient method to simulate systems involving distributions of parameters, and works equally well in three spatial dimensions. One limitation is that the choice of polynomials depends on type of distribution assumed for the parameters. However, this choice only affects the definition of the matrix M. Also, one needs appropriate error estimates to be sure that a sufficient number of polynomials is used in the expansion. However, as the matrix does not change over time steps, the complexity of solving for the random polarization scales linearly with the number of terms in the expansion, while the error decays exponentially [4].

Inverse Problem Numerical Results

In Figure 2 we show a plot of time domain electric field data with 20% random noise added. This data was simulated using the Beta distribution of relaxation times depicted in Figure 3. Note that the shape of Beta distribution can mimic a log-normal, but with finite support, thus is it especially appropriate for use in multi-pole models. Given the data, a nonlinear least squares inverse problem for the shape parameters of the Beta distribution was solved using as an initial guess the distribution also depicted in Figure 3. It is clear that the forward simulation corresponding to this initial distribution is significantly different from the data, as shown in Figure 2. The optimal distribution found is indistinguishable from the actual (see Figure 3); likewise the corresponding forward simulation matches a simulation performed using the actual distribution (see Figure 2).

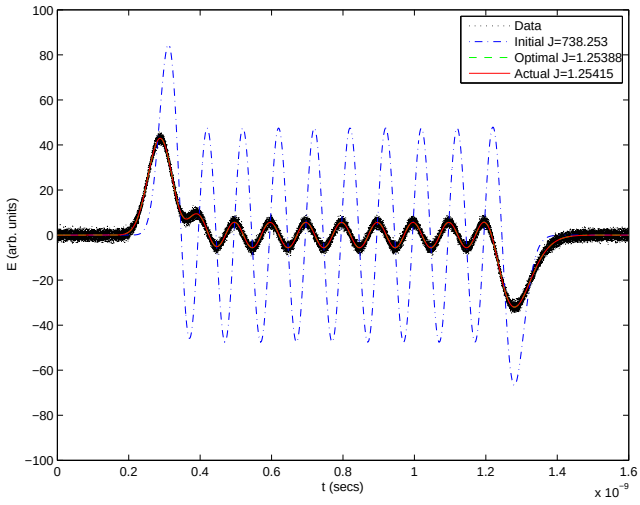

Figure 2: Comparison of simulations to data.

Conclusion

Previous work showed that estimation approach for distributions worked well given time domain electric field data [2]. We have improved on the accuracy and speed of the forward simulations [6], [4]. We are now able to efficiently determine the shape of the Beta distributions with confidence in spite of noise. Similar results have been obtained with very broad bandwith signal and with combining multiple polarization mechinisms.

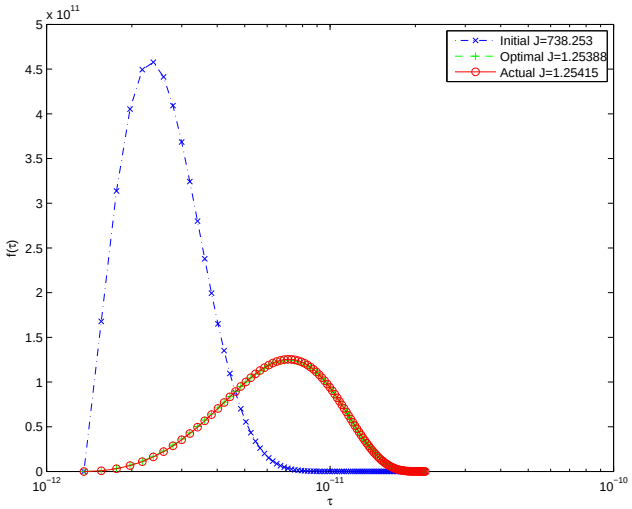

Figure 3: Comparing initial to final distribution.

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