Polynomial Chaos Approach for Simulations in Dispersive Media

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Outline

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   - Polarization Models
   - Distribution of Relaxation Times
2. Polynomial Chaos
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   - Galerkin Projection
3. Discretization
   - The Yee Scheme
   - Time Discretization of PC Solution
   - Stability Analysis
   - Numerical Simulations

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H} \qquad \text{(Ampere)}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \text{(Faraday)}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Poisson)}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss)}$$

$\mathbf{E} =$ Electric field vector $\qquad$ $\mathbf{D} =$ Electric displacement

$\mathbf{H} =$ Magnetic field vector $\qquad$ $\mathbf{B} =$ Magnetic flux density

$\rho =$ Electric charge density $\qquad$ $\mathbf{J} =$ Current density

With appropriate initial conditions and boundary conditions.

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$
$$\mathbf{B} = \mu \mathbf{H} + \mathbf{M}$$
$$\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_s$$

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Complex permittivity

- We can define $\mathbf{P}$ in terms of a convolution

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

  where g is the dielectric response function (DRF).
- In the frequency domain $\hat{\mathbf{D}} = \epsilon_0 \epsilon(\omega)\hat{\mathbf{E}}$, where $\epsilon(\omega)$ is called the complex permittivity.
- $\epsilon(\omega)$ described by the polarization model (and conductivity)
- We are interested in ultra-wide bandwidth electromagnetic pulse interrogation of dispersive dielectrics, therefore we want an accurate representation of $\epsilon(\omega)$ over a broad range of frequencies.

Dispersive Media

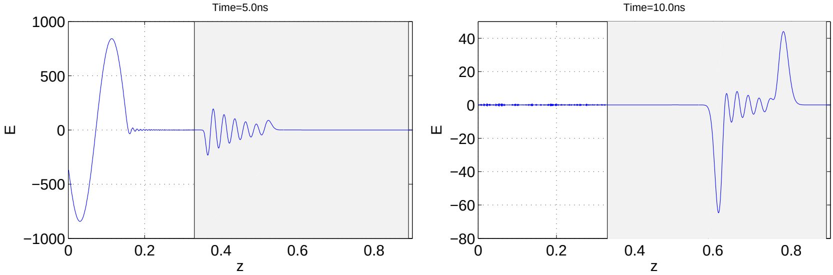

Figure: Debye model simulations.

Dry skin data

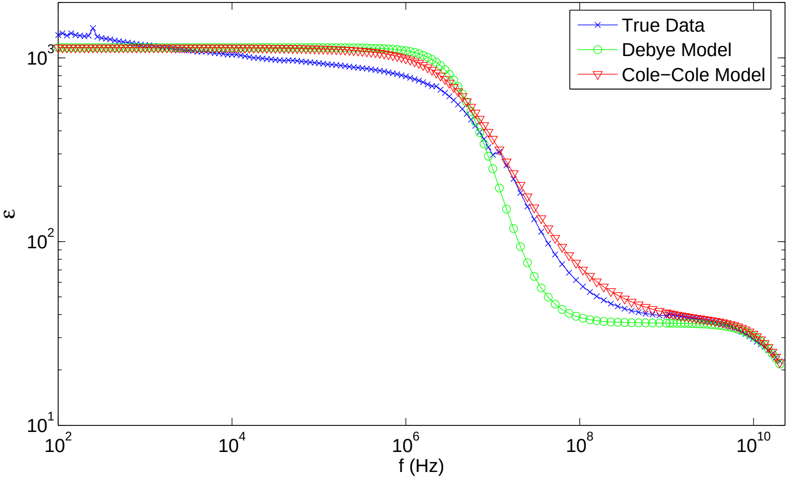

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

Dry skin data

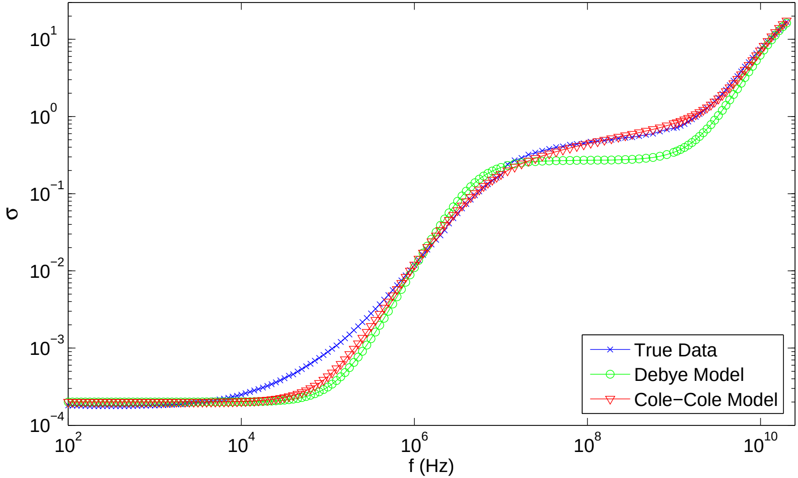

Figure: Imaginary part of $\epsilon(\omega)$, σ, or the conductivity.

Sample models

- Debye model [1929] $\mathbf{q} = [\epsilon_d, \tau]$

$$g(t, \mathbf{x}) = \epsilon_0 \epsilon_d / \tau \quad e^{-t/\tau}$$

$$\text{or} \quad \tau \dot{\mathbf{P}} + \mathbf{P} = \epsilon_0 \epsilon_d \mathbf{E}$$

$$\text{or} \quad \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + i\omega\tau}$$

with $\epsilon_d := \epsilon_0(\epsilon_s - \epsilon_\infty)$.

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  with $\epsilon_d := \epsilon_0(\epsilon_s - \epsilon_\infty)$.

- Cole-Cole model [1936] (heuristic generalization) $\mathbf{q} = [\epsilon_d, \tau, \alpha]$

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1 + (i\omega\tau)^{1-\alpha}}$$

Motivation

- Broadband wave propagation suggests time-domain simulation.
- The Cole-Cole model corresponds to a fractional order ODE in the time-domain and is difficult to simulate.
- Debye is efficient to simulate, but does not represent permittivity well.
- Better fits to data are obtained by taking linear combinations of Debye models (discrete distributions), idea comes from the known existence of multiple physical mechanisms.
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times [von Schweidler1907].
- Empirical measurements suggest a log-normal distribution [Wagner1913], but uniform is easier.

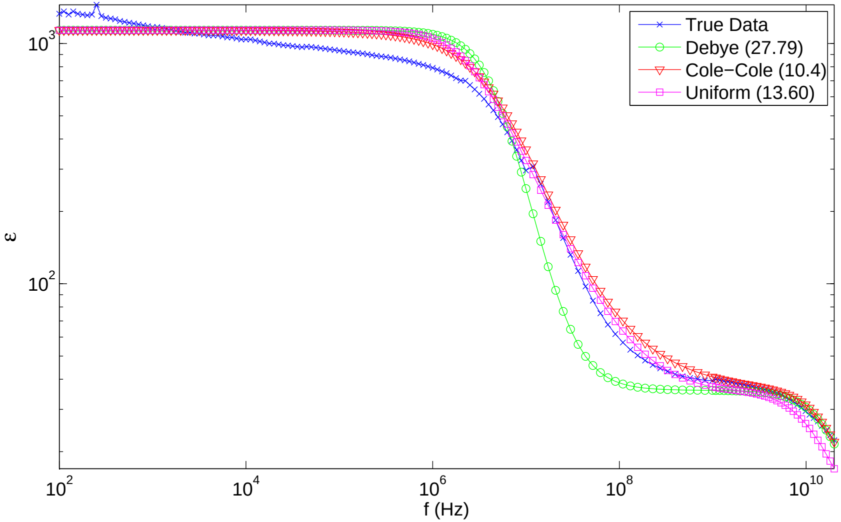


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

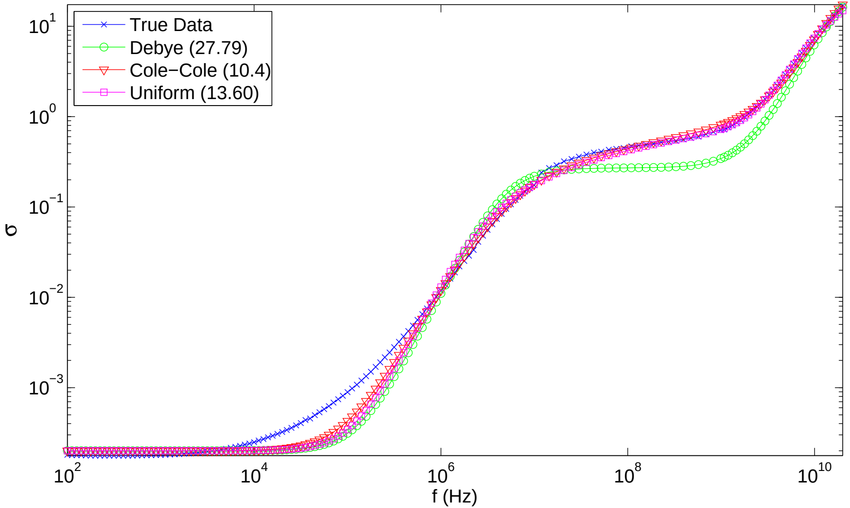


Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

To account for the effect of possible multiple parameter sets $\mathbf{q}$, consider

$$h(t, \mathbf{x}; F) = \int_{\mathcal{Q}} g(t, \mathbf{x}; \mathbf{q}) dF(\mathbf{q}),$$

where $\mathcal{Q}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{Q})$.
Then the polarization becomes:

$$\mathbf{P}(t, \mathbf{x}) = \int_0^t h(t - s, \mathbf{x}; F)\mathbf{E}(s, \mathbf{x}) ds.$$

The inverse problem for F given time domain electric field data is well-posed [BG05, BG06].

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

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d \mathbf{E}$$

where τ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.
The electric field depends on the macroscopic polarization, which we take to be the expected value of the stochastic polarization at each point $(t, \mathbf{x})$

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

We can apply the generalized Polynomial Chaos method [XK03] to the *random ordinary differential equation* (at each point in space and each dimension independently)

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d E, \quad \tau = \tau(\xi) = \tau_\sigma\xi + \tau_\mu$$

where $\xi \sim U(-1,1)$, for example.
We apply a Polynomial Chaos expansion in terms of orthogonal polynomials $\phi_j(\xi)$ to the solution $\mathcal{P}$:

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

The RODE becomes

$$(\tau_\sigma\xi + \tau_\mu)\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi) = \epsilon_d E.$$

$$(\tau_\sigma \xi + \tau_\mu) \sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) + \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi) = \epsilon_d E$$

We can eliminate the explicit dependence on ξ by using the triple recursion formula for orthogonal polynomials

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

(with $\phi_{-1} = 0$), for example, for Legendre polynomials

$$(2j+1)\xi\phi_j = j\phi_{j-1} + (j+1)\phi_{j+1}.$$

In general, the RODE becomes

$$\tau_\sigma \sum_{j=0}^{\infty} \dot{\alpha}_j(t)(a_j\phi_{j-1} + b_j\phi_j + c_j\phi_{j+1}) + \tau_\mu \sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j + \sum_{j=0}^{\infty} \alpha_j(t)\phi_j = \epsilon_d E.$$

We take the weighted inner product with each basis $\{\phi_j\}_{j=0}^p$ for a fixed p resulting in the approximating system

$$(\tau_\sigma M + \tau_\mu I)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_d E \vec{e}_1,$$

where $\vec{\alpha} = [\alpha_0(t), \ldots, \alpha_p(t)]^T$ and

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

or, more simply,

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

The macroscopic polarization is taken to be the expected value of the stochastic polarization at each point $(t, \mathbf{x})$, for each dimension

$$P(t, \mathbf{x}) = \mathcal{E}[\mathcal{P}(t, \mathbf{x})] \approx \alpha_0(t, \mathbf{x}).$$

Exponential convergence

- Any set of orthogonal polynomials can be used in the truncated expansion, but there may be an optimal choice.
- If the polynomials are orthogonal with respect to weighting function $f(\xi)$, and k has PDF $f(k)$, then it is known that the PC solution to the ODE converges exponentially in terms of p.
- In practice, approximately 4 are generally sufficient.

Generalized Polynomial Chaos

Table: Popular distributions and corresponding orthogonal polynomials.

Distribution	Polynomial	Support
Gaussian	Hermite	$(-\infty, \infty)$
gamma	Laguerre	$[0, \infty)$
beta	Jacobi	$[a, b]$
uniform	Legendre	$[a, b]$

Note: log-normal random variables may be handled as a non-linear function (e.g., Taylor expansion) of a normal random variable.

Existence of PC Solutions

Theorem (REU2010)

For the beta-Jacobi chaos (including uniform-Legendre), there exists solutions to the system

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

for any p.

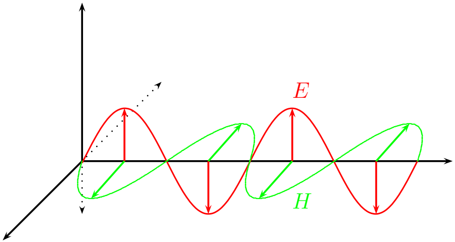
Proof.

Relies on the fact that the invertibility of A requires $\tau_\mu > \tau_\sigma$. This is physically reasonable as to disallow negative relaxation times. □

- Assume uniformity in the x-direction.
- Assume that the electric field is polarized to oscillate only in the y direction.

Evolution equations involving E, H, D, B, P and J:

$$\frac{\partial D}{\partial t} + J = \frac{\partial H}{\partial z}$$
$$\frac{\partial B}{\partial t} = \frac{\partial E}{\partial z}$$



Constitutive laws:

$$B = \mu H$$
$$D = \epsilon E + P$$
$$J = \sigma E + J_s$$

Applying the central difference approximation, based on the Yee scheme, our one dimensional equations

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

and

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

become

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

and

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

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

We discretize the PC system

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

by applying central differences to $\vec{\alpha} = \vec{\alpha}(z_k)$ for arbitrary z_k

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

Combining like terms gives

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

Note that we may first solve the discrete electric field equation for $E_k^{n+\frac{1}{2}}$ and plug into $\vec{g}^{n+\frac{1}{2}}$ to define a decoupled update step for $\vec{\alpha}$.

Stability Analysis

We look for plane wave solutions and assume spatial dependence of the form

$$
\begin{aligned}
H_{j+\frac{1}{2}}^{n+1} &= \hat{H}^{n+1}(k)\mathrm{e}^{\mathrm{i}k(j+\frac{1}{2})\Delta z} \\
E_{j}^{n+\frac{1}{2}} &= \hat{E}^{n+\frac{1}{2}}(k)\mathrm{e}^{\mathrm{i}kj\Delta z} \\
\alpha_{0,j}^{n+\frac{1}{2}} &= \hat{\alpha}_{0}^{n+\frac{1}{2}}(k)\mathrm{e}^{\mathrm{i}kj\Delta z} \\
&\vdots \\
\alpha_{p,j}^{n+\frac{1}{2}} &= \hat{\alpha}_{p}^{n+\frac{1}{2}}(k)\mathrm{e}^{\mathrm{i}kj\Delta z}
\end{aligned}
$$

where k is the wave number.

Substituting the above into our numerical method we obtain

$$BU^{n+1} = CU^n$$

where

$$U^n := [\hat{H}^n, \hat{E}^{n+\frac{1}{2}}, \hat{\alpha_0}^{n+\frac{1}{2}}, \ldots, \hat{\alpha_p}^{n+\frac{1}{2}}]$$

$$B := \begin{bmatrix} B_{11} & B_{12}^T \\ B_{21} & 2A + \Delta t I \end{bmatrix} \qquad B11 := \begin{bmatrix} 1 & \gamma/\mu \\ 0 & \theta^+ \end{bmatrix}$$

$$B12 := \begin{bmatrix} 0 & 2 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix} \qquad B21 := \begin{bmatrix} 0 & -\Delta t\, \epsilon_d \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}$$

$$\theta^+ := 2\epsilon + \sigma\Delta t \qquad \gamma := \frac{2\mathrm{i}\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)$$

Continuing:

$$BU^{n+1} = CU^n$$

where

$$B := \begin{bmatrix} B_{11} & B_{12}^T \\ B_{21} & 2A + \Delta t I \end{bmatrix} \qquad B11 := \begin{bmatrix} 1 & \gamma/\mu \\ 0 & \theta^+ \end{bmatrix}$$

$$C := \begin{bmatrix} C_{11} & B_{12}^T \\ -B_{21} & 2A - \Delta t I \end{bmatrix} \qquad C11 := \begin{bmatrix} 1 & 0 \\ -2\gamma & \theta^- \end{bmatrix}$$

$$\theta^+ := 2\epsilon + \sigma\Delta t \qquad \theta^- := 2\epsilon - \sigma\Delta t$$

$$\gamma := \frac{2\mathrm{i}\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)$$

Note: for $p = 0$, $A = \tau_\mu$ and we recover single Debye equations.

Stability of uniform-Legendre Chaos system

Theorem (REU2010)

The numerical polynomial chaos scheme is stable for Legendre polynomials with $p = 1$ if and only if the following conditions hold

$$\nu \leq 1$$
$$\epsilon_s \geq \epsilon_\infty$$
$$\tau_\mu \geq 0.$$

Proof.

Direct application of Routh-Horwitz criteria □

The last condition again disallows negative relaxation times.

Numerical Stability Analysis

- If the modulus of all the generalized (complex, time) eigenvalues of (B, C) are less than one, the method is stable.
- The stability polynomial given by $\det(C - \lambda B)$ is of degree $p + 3$.
- The roots depend on material and discretization parameters including: $k\Delta z$ (quantifies ppw), $h := \Delta t/\tau_\mu$ (temporal resolution), ν (relates Δz and Δt), as well as τ_σ (quantifies variance).
- We plot the largest modulus of λ as a function of $k\Delta z$ in the following with all other parameters fixed.

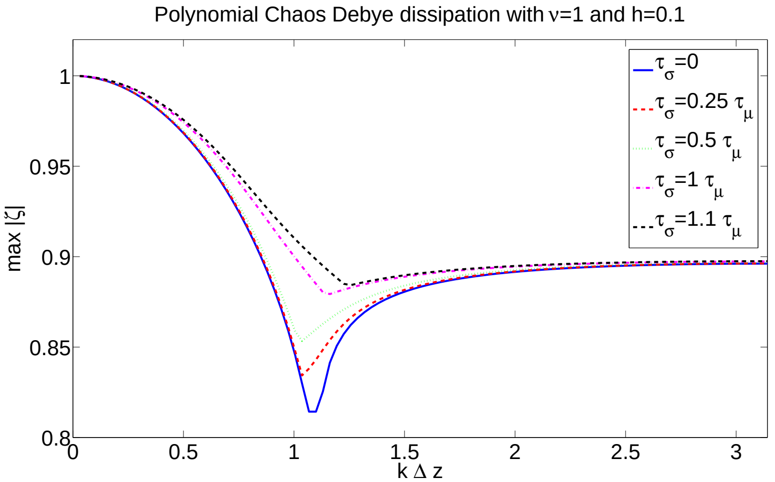


Figure: Using parameters of dry skin data and $p = 2$

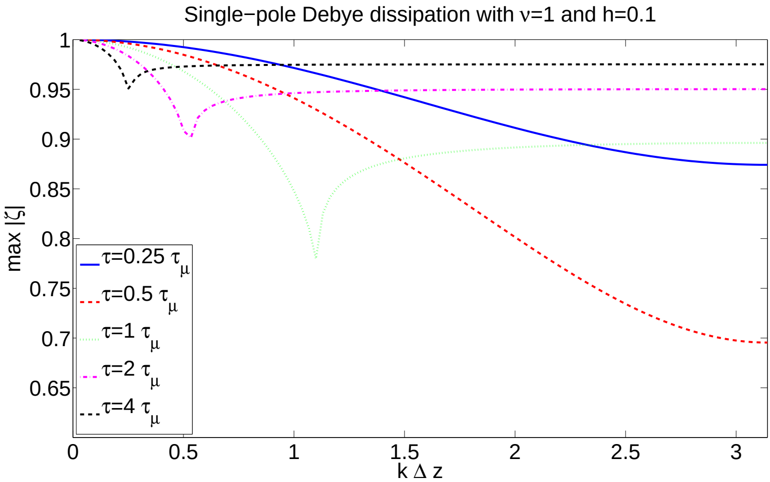
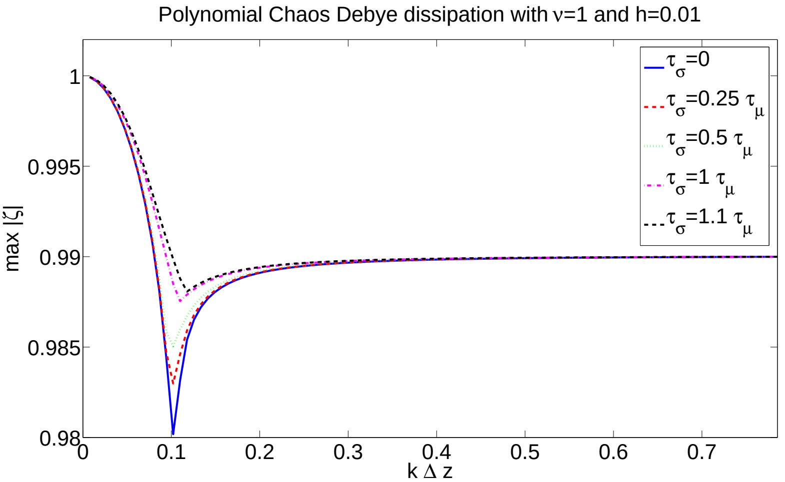


Figure: Using parameters of dry skin data and $p = 0$



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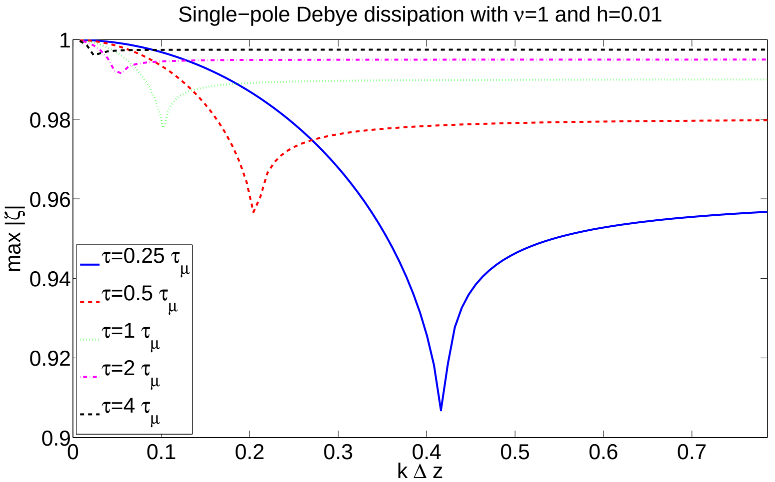

Figure: Using parameters of dry skin data and $p = 0$

Numerical Simulations

- Windowed 10^{10} Hz signal propagation in a stochastic Debye dielectric model of water.
- Time trace measured at 0.015 m inside material.
- Let $h_\tau := \Delta t/\tau_\mu$, where $\tau_\mu = 8.13 \times 10^{-12}$ is the measured deterministic value.
- We use Uniform-Legendre chaos expansions with, for example, $\tau \sim U[.75\tau_\mu, 1.25\tau_\mu]$.

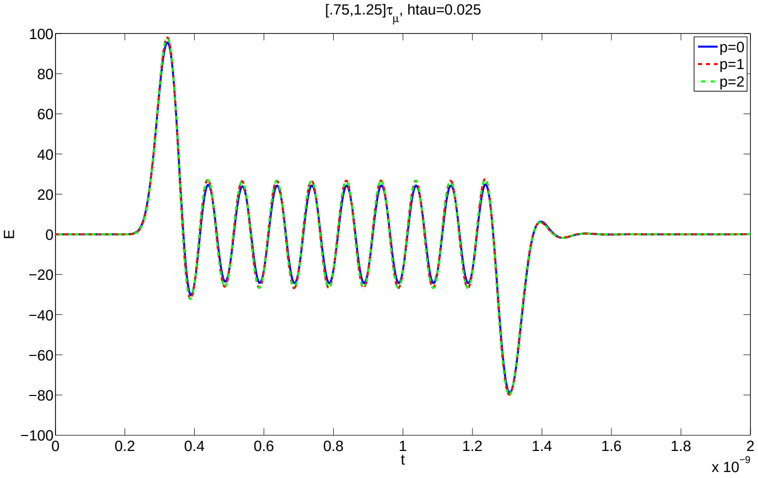

Figure: Using parameters of dry skin data with $\tau \sim U[.75\tau_\mu, 1.25\tau_\mu]$, and using $p = 0, 1, 2$ polynomials. Shows significant convergence after just $p = 1$.

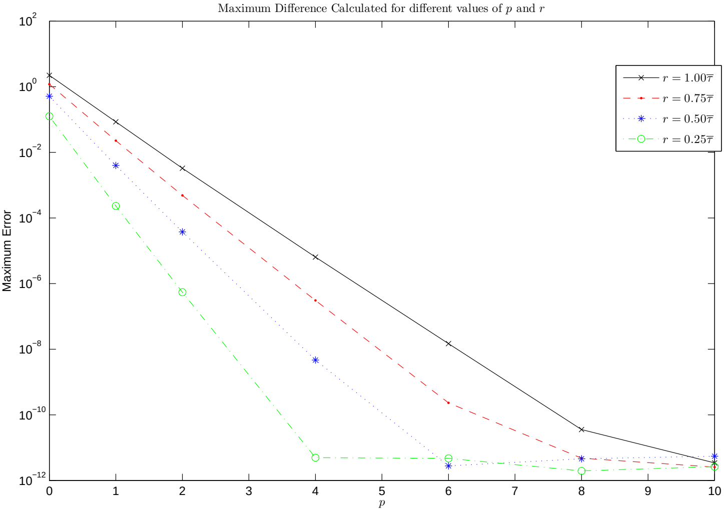

Figure: Maximum Error for various values of p and r.

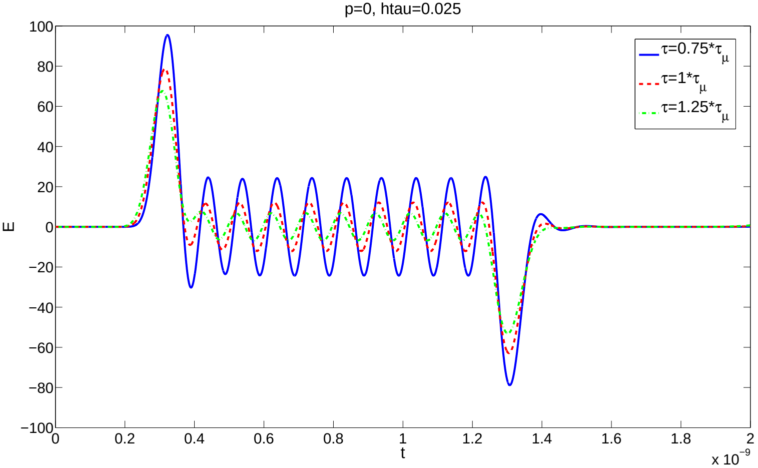

Figure: Using parameters of dry skin data with deterministic $\tau \in [.75\tau_\mu, 1.25\tau_\mu]$. Shows suggests that stochastic polarization will have slightly higher amplitude if considered as an average of these simulations.

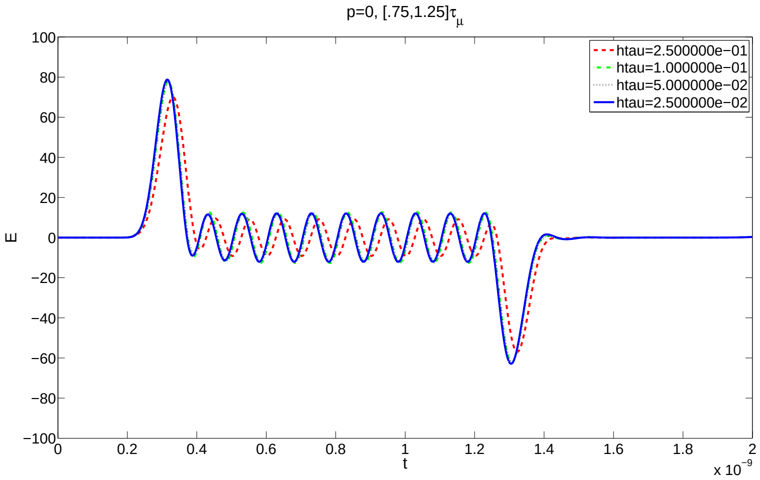

Figure: Using parameters of dry skin data and $p = 0$. Shows $h_\tau = 0.01$ required for accuracy.

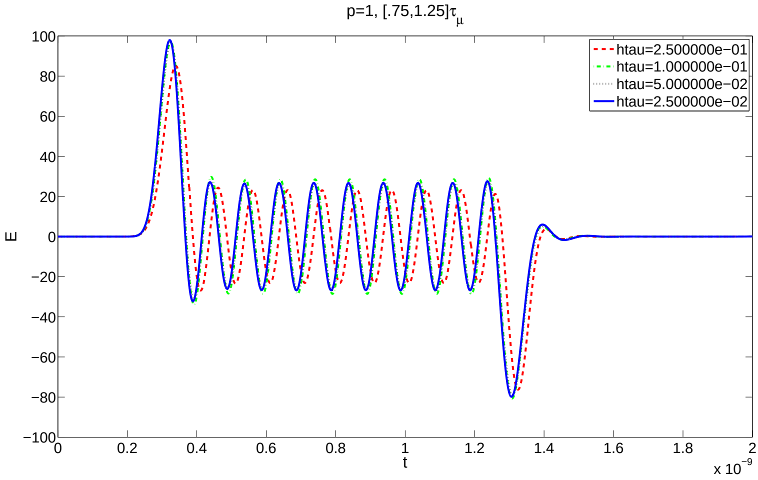

Figure: Using parameters of dry skin data and $p = 1$. Shows $h_\tau = 0.005$ required for accuracy. Non-zero variance implies smaller relaxation times are present.

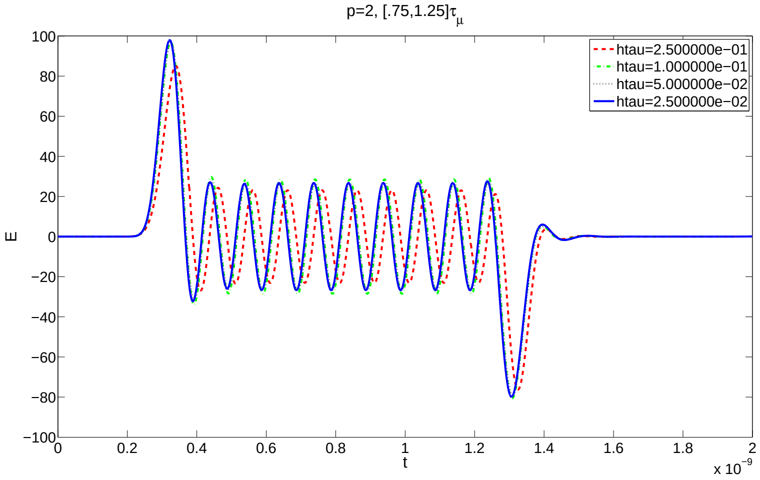

Figure: Using parameters of dry skin data and $p = 2$. Shows $h_\tau = 0.005$ required for accuracy. As expected, including more polynomials does not reduce temporal resolution errors.

Conclusions

- Stochastic Polarization well suited for modeling realistic dielectric materials
- Distributions of parameters avoids fractional order derivative models
- Polynomial Chaos is a simple-to-use method for efficiently simulating stochastic polarization
- Stability properties of the numerical method are similar to deterministic case
- Stochastic polarization exhibits less dissipation for comparable discretization parameters

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